



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 12:21 AM UTC

PDB ID : 9RQT / pdb_00009rqt
EMDB ID : EMD-54184
Title : Heptameric AAV2 Rep40-dsDNA (ITR) complex in presence of ATPgS
Authors : Rouse, S.L.; Bubeck, D.; Barritt, J.D.; Xu, V.; Wake, M.
Deposited on : 2025-06-26
Resolution : 2.88 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

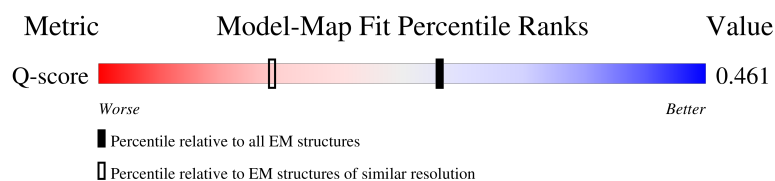
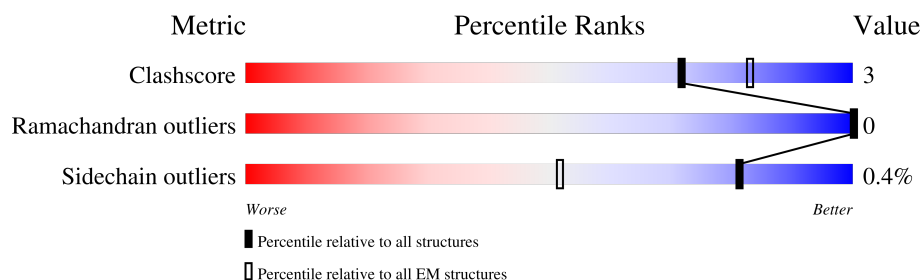
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	145	 19% 81%
2	a	397	 67% 30%
2	b	397	 68% 30%
2	c	397	 67% 30%

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Mol	Chain	Length	Quality of chain
2	d	397	<div><div></div><div>65%5%30%</div></div>
2	e	397	<div><div></div><div>61%7%31%</div></div>
2	f	397	<div><div></div><div>59%9%31%</div></div>
2	g	397	<div><div></div><div>62%6%31%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16036 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 DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	28	Total	C	N	O	P	0	0
			574	269	109	168	28		

- Molecule 2 is a protein called Protein Rep40.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	278	Total	C	N	O	S	0	0
			2214	1410	378	416	10		
2	b	278	Total	C	N	O	S	0	0
			2214	1410	378	416	10		
2	c	278	Total	C	N	O	S	0	0
			2214	1410	378	416	10		
2	d	277	Total	C	N	O	S	0	0
			2210	1408	377	415	10		
2	e	273	Total	C	N	O	S	0	0
			2175	1387	370	409	9		
2	f	272	Total	C	N	O	S	0	0
			2173	1387	369	408	9		
2	g	272	Total	C	N	O	S	0	0
			2170	1385	369	407	9		

There are 595 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	GLU	-	expression tag	UNP Q89269
a	2	GLN	-	expression tag	UNP Q89269
a	3	ASN	-	expression tag	UNP Q89269
a	4	LYS	-	expression tag	UNP Q89269
a	5	GLU	-	expression tag	UNP Q89269
a	6	ASN	-	expression tag	UNP Q89269
a	7	GLN	-	expression tag	UNP Q89269
a	8	ASN	-	expression tag	UNP Q89269
a	9	PRO	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
a	10	ASN	-	expression tag	UNP Q89269
a	11	SER	-	expression tag	UNP Q89269
a	12	ASP	-	expression tag	UNP Q89269
a	13	ALA	-	expression tag	UNP Q89269
a	14	PRO	-	expression tag	UNP Q89269
a	15	VAL	-	expression tag	UNP Q89269
a	16	ILE	-	expression tag	UNP Q89269
a	17	ARG	-	expression tag	UNP Q89269
a	18	SER	-	expression tag	UNP Q89269
a	19	LYS	-	expression tag	UNP Q89269
a	20	THR	-	expression tag	UNP Q89269
a	21	SER	-	expression tag	UNP Q89269
a	22	ALA	-	expression tag	UNP Q89269
a	23	ARG	-	expression tag	UNP Q89269
a	24	TYR	-	expression tag	UNP Q89269
a	337	GLY	-	expression tag	UNP Q89269
a	338	SER	-	expression tag	UNP Q89269
a	339	LEU	-	expression tag	UNP Q89269
a	340	VAL	-	expression tag	UNP Q89269
a	341	PRO	-	expression tag	UNP Q89269
a	342	ARG	-	expression tag	UNP Q89269
a	343	GLY	-	expression tag	UNP Q89269
a	344	SER	-	expression tag	UNP Q89269
a	345	GLY	-	expression tag	UNP Q89269
a	346	GLY	-	expression tag	UNP Q89269
a	347	GLY	-	expression tag	UNP Q89269
a	348	GLY	-	expression tag	UNP Q89269
a	349	SER	-	expression tag	UNP Q89269
a	350	GLY	-	expression tag	UNP Q89269
a	351	GLY	-	expression tag	UNP Q89269
a	352	GLY	-	expression tag	UNP Q89269
a	353	GLY	-	expression tag	UNP Q89269
a	354	SER	-	expression tag	UNP Q89269
a	355	GLY	-	expression tag	UNP Q89269
a	356	GLY	-	expression tag	UNP Q89269
a	357	GLY	-	expression tag	UNP Q89269
a	358	GLY	-	expression tag	UNP Q89269
a	359	SER	-	expression tag	UNP Q89269
a	360	MET	-	expression tag	UNP Q89269
a	361	ASP	-	expression tag	UNP Q89269
a	362	TYR	-	expression tag	UNP Q89269
a	363	LYS	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
a	364	ASP	-	expression tag	UNP Q89269
a	365	HIS	-	expression tag	UNP Q89269
a	366	ASP	-	expression tag	UNP Q89269
a	367	GLY	-	expression tag	UNP Q89269
a	368	ASP	-	expression tag	UNP Q89269
a	369	TYR	-	expression tag	UNP Q89269
a	370	LYS	-	expression tag	UNP Q89269
a	371	ASP	-	expression tag	UNP Q89269
a	372	HIS	-	expression tag	UNP Q89269
a	373	ASP	-	expression tag	UNP Q89269
a	374	ILE	-	expression tag	UNP Q89269
a	375	ASP	-	expression tag	UNP Q89269
a	376	TYR	-	expression tag	UNP Q89269
a	377	LYS	-	expression tag	UNP Q89269
a	378	ASP	-	expression tag	UNP Q89269
a	379	ASP	-	expression tag	UNP Q89269
a	380	ASP	-	expression tag	UNP Q89269
a	381	ASP	-	expression tag	UNP Q89269
a	382	LYS	-	expression tag	UNP Q89269
a	383	GLY	-	expression tag	UNP Q89269
a	384	SER	-	expression tag	UNP Q89269
a	385	GLU	-	expression tag	UNP Q89269
a	386	ASN	-	expression tag	UNP Q89269
a	387	LEU	-	expression tag	UNP Q89269
a	388	TYR	-	expression tag	UNP Q89269
a	389	PHE	-	expression tag	UNP Q89269
a	390	GLN	-	expression tag	UNP Q89269
a	391	SER	-	expression tag	UNP Q89269
a	392	HIS	-	expression tag	UNP Q89269
a	393	HIS	-	expression tag	UNP Q89269
a	394	HIS	-	expression tag	UNP Q89269
a	395	HIS	-	expression tag	UNP Q89269
a	396	HIS	-	expression tag	UNP Q89269
a	397	HIS	-	expression tag	UNP Q89269
b	1	GLU	-	expression tag	UNP Q89269
b	2	GLN	-	expression tag	UNP Q89269
b	3	ASN	-	expression tag	UNP Q89269
b	4	LYS	-	expression tag	UNP Q89269
b	5	GLU	-	expression tag	UNP Q89269
b	6	ASN	-	expression tag	UNP Q89269
b	7	GLN	-	expression tag	UNP Q89269
b	8	ASN	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
b	9	PRO	-	expression tag	UNP Q89269
b	10	ASN	-	expression tag	UNP Q89269
b	11	SER	-	expression tag	UNP Q89269
b	12	ASP	-	expression tag	UNP Q89269
b	13	ALA	-	expression tag	UNP Q89269
b	14	PRO	-	expression tag	UNP Q89269
b	15	VAL	-	expression tag	UNP Q89269
b	16	ILE	-	expression tag	UNP Q89269
b	17	ARG	-	expression tag	UNP Q89269
b	18	SER	-	expression tag	UNP Q89269
b	19	LYS	-	expression tag	UNP Q89269
b	20	THR	-	expression tag	UNP Q89269
b	21	SER	-	expression tag	UNP Q89269
b	22	ALA	-	expression tag	UNP Q89269
b	23	ARG	-	expression tag	UNP Q89269
b	24	TYR	-	expression tag	UNP Q89269
b	337	GLY	-	expression tag	UNP Q89269
b	338	SER	-	expression tag	UNP Q89269
b	339	LEU	-	expression tag	UNP Q89269
b	340	VAL	-	expression tag	UNP Q89269
b	341	PRO	-	expression tag	UNP Q89269
b	342	ARG	-	expression tag	UNP Q89269
b	343	GLY	-	expression tag	UNP Q89269
b	344	SER	-	expression tag	UNP Q89269
b	345	GLY	-	expression tag	UNP Q89269
b	346	GLY	-	expression tag	UNP Q89269
b	347	GLY	-	expression tag	UNP Q89269
b	348	GLY	-	expression tag	UNP Q89269
b	349	SER	-	expression tag	UNP Q89269
b	350	GLY	-	expression tag	UNP Q89269
b	351	GLY	-	expression tag	UNP Q89269
b	352	GLY	-	expression tag	UNP Q89269
b	353	GLY	-	expression tag	UNP Q89269
b	354	SER	-	expression tag	UNP Q89269
b	355	GLY	-	expression tag	UNP Q89269
b	356	GLY	-	expression tag	UNP Q89269
b	357	GLY	-	expression tag	UNP Q89269
b	358	GLY	-	expression tag	UNP Q89269
b	359	SER	-	expression tag	UNP Q89269
b	360	MET	-	expression tag	UNP Q89269
b	361	ASP	-	expression tag	UNP Q89269
b	362	TYR	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
b	363	LYS	-	expression tag	UNP Q89269
b	364	ASP	-	expression tag	UNP Q89269
b	365	HIS	-	expression tag	UNP Q89269
b	366	ASP	-	expression tag	UNP Q89269
b	367	GLY	-	expression tag	UNP Q89269
b	368	ASP	-	expression tag	UNP Q89269
b	369	TYR	-	expression tag	UNP Q89269
b	370	LYS	-	expression tag	UNP Q89269
b	371	ASP	-	expression tag	UNP Q89269
b	372	HIS	-	expression tag	UNP Q89269
b	373	ASP	-	expression tag	UNP Q89269
b	374	ILE	-	expression tag	UNP Q89269
b	375	ASP	-	expression tag	UNP Q89269
b	376	TYR	-	expression tag	UNP Q89269
b	377	LYS	-	expression tag	UNP Q89269
b	378	ASP	-	expression tag	UNP Q89269
b	379	ASP	-	expression tag	UNP Q89269
b	380	ASP	-	expression tag	UNP Q89269
b	381	ASP	-	expression tag	UNP Q89269
b	382	LYS	-	expression tag	UNP Q89269
b	383	GLY	-	expression tag	UNP Q89269
b	384	SER	-	expression tag	UNP Q89269
b	385	GLU	-	expression tag	UNP Q89269
b	386	ASN	-	expression tag	UNP Q89269
b	387	LEU	-	expression tag	UNP Q89269
b	388	TYR	-	expression tag	UNP Q89269
b	389	PHE	-	expression tag	UNP Q89269
b	390	GLN	-	expression tag	UNP Q89269
b	391	SER	-	expression tag	UNP Q89269
b	392	HIS	-	expression tag	UNP Q89269
b	393	HIS	-	expression tag	UNP Q89269
b	394	HIS	-	expression tag	UNP Q89269
b	395	HIS	-	expression tag	UNP Q89269
b	396	HIS	-	expression tag	UNP Q89269
b	397	HIS	-	expression tag	UNP Q89269
c	1	GLU	-	expression tag	UNP Q89269
c	2	GLN	-	expression tag	UNP Q89269
c	3	ASN	-	expression tag	UNP Q89269
c	4	LYS	-	expression tag	UNP Q89269
c	5	GLU	-	expression tag	UNP Q89269
c	6	ASN	-	expression tag	UNP Q89269
c	7	GLN	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
c	8	ASN	-	expression tag	UNP Q89269
c	9	PRO	-	expression tag	UNP Q89269
c	10	ASN	-	expression tag	UNP Q89269
c	11	SER	-	expression tag	UNP Q89269
c	12	ASP	-	expression tag	UNP Q89269
c	13	ALA	-	expression tag	UNP Q89269
c	14	PRO	-	expression tag	UNP Q89269
c	15	VAL	-	expression tag	UNP Q89269
c	16	ILE	-	expression tag	UNP Q89269
c	17	ARG	-	expression tag	UNP Q89269
c	18	SER	-	expression tag	UNP Q89269
c	19	LYS	-	expression tag	UNP Q89269
c	20	THR	-	expression tag	UNP Q89269
c	21	SER	-	expression tag	UNP Q89269
c	22	ALA	-	expression tag	UNP Q89269
c	23	ARG	-	expression tag	UNP Q89269
c	24	TYR	-	expression tag	UNP Q89269
c	337	GLY	-	expression tag	UNP Q89269
c	338	SER	-	expression tag	UNP Q89269
c	339	LEU	-	expression tag	UNP Q89269
c	340	VAL	-	expression tag	UNP Q89269
c	341	PRO	-	expression tag	UNP Q89269
c	342	ARG	-	expression tag	UNP Q89269
c	343	GLY	-	expression tag	UNP Q89269
c	344	SER	-	expression tag	UNP Q89269
c	345	GLY	-	expression tag	UNP Q89269
c	346	GLY	-	expression tag	UNP Q89269
c	347	GLY	-	expression tag	UNP Q89269
c	348	GLY	-	expression tag	UNP Q89269
c	349	SER	-	expression tag	UNP Q89269
c	350	GLY	-	expression tag	UNP Q89269
c	351	GLY	-	expression tag	UNP Q89269
c	352	GLY	-	expression tag	UNP Q89269
c	353	GLY	-	expression tag	UNP Q89269
c	354	SER	-	expression tag	UNP Q89269
c	355	GLY	-	expression tag	UNP Q89269
c	356	GLY	-	expression tag	UNP Q89269
c	357	GLY	-	expression tag	UNP Q89269
c	358	GLY	-	expression tag	UNP Q89269
c	359	SER	-	expression tag	UNP Q89269
c	360	MET	-	expression tag	UNP Q89269
c	361	ASP	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
c	362	TYR	-	expression tag	UNP Q89269
c	363	LYS	-	expression tag	UNP Q89269
c	364	ASP	-	expression tag	UNP Q89269
c	365	HIS	-	expression tag	UNP Q89269
c	366	ASP	-	expression tag	UNP Q89269
c	367	GLY	-	expression tag	UNP Q89269
c	368	ASP	-	expression tag	UNP Q89269
c	369	TYR	-	expression tag	UNP Q89269
c	370	LYS	-	expression tag	UNP Q89269
c	371	ASP	-	expression tag	UNP Q89269
c	372	HIS	-	expression tag	UNP Q89269
c	373	ASP	-	expression tag	UNP Q89269
c	374	ILE	-	expression tag	UNP Q89269
c	375	ASP	-	expression tag	UNP Q89269
c	376	TYR	-	expression tag	UNP Q89269
c	377	LYS	-	expression tag	UNP Q89269
c	378	ASP	-	expression tag	UNP Q89269
c	379	ASP	-	expression tag	UNP Q89269
c	380	ASP	-	expression tag	UNP Q89269
c	381	ASP	-	expression tag	UNP Q89269
c	382	LYS	-	expression tag	UNP Q89269
c	383	GLY	-	expression tag	UNP Q89269
c	384	SER	-	expression tag	UNP Q89269
c	385	GLU	-	expression tag	UNP Q89269
c	386	ASN	-	expression tag	UNP Q89269
c	387	LEU	-	expression tag	UNP Q89269
c	388	TYR	-	expression tag	UNP Q89269
c	389	PHE	-	expression tag	UNP Q89269
c	390	GLN	-	expression tag	UNP Q89269
c	391	SER	-	expression tag	UNP Q89269
c	392	HIS	-	expression tag	UNP Q89269
c	393	HIS	-	expression tag	UNP Q89269
c	394	HIS	-	expression tag	UNP Q89269
c	395	HIS	-	expression tag	UNP Q89269
c	396	HIS	-	expression tag	UNP Q89269
c	397	HIS	-	expression tag	UNP Q89269
d	1	GLU	-	expression tag	UNP Q89269
d	2	GLN	-	expression tag	UNP Q89269
d	3	ASN	-	expression tag	UNP Q89269
d	4	LYS	-	expression tag	UNP Q89269
d	5	GLU	-	expression tag	UNP Q89269
d	6	ASN	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
d	7	GLN	-	expression tag	UNP Q89269
d	8	ASN	-	expression tag	UNP Q89269
d	9	PRO	-	expression tag	UNP Q89269
d	10	ASN	-	expression tag	UNP Q89269
d	11	SER	-	expression tag	UNP Q89269
d	12	ASP	-	expression tag	UNP Q89269
d	13	ALA	-	expression tag	UNP Q89269
d	14	PRO	-	expression tag	UNP Q89269
d	15	VAL	-	expression tag	UNP Q89269
d	16	ILE	-	expression tag	UNP Q89269
d	17	ARG	-	expression tag	UNP Q89269
d	18	SER	-	expression tag	UNP Q89269
d	19	LYS	-	expression tag	UNP Q89269
d	20	THR	-	expression tag	UNP Q89269
d	21	SER	-	expression tag	UNP Q89269
d	22	ALA	-	expression tag	UNP Q89269
d	23	ARG	-	expression tag	UNP Q89269
d	24	TYR	-	expression tag	UNP Q89269
d	337	GLY	-	expression tag	UNP Q89269
d	338	SER	-	expression tag	UNP Q89269
d	339	LEU	-	expression tag	UNP Q89269
d	340	VAL	-	expression tag	UNP Q89269
d	341	PRO	-	expression tag	UNP Q89269
d	342	ARG	-	expression tag	UNP Q89269
d	343	GLY	-	expression tag	UNP Q89269
d	344	SER	-	expression tag	UNP Q89269
d	345	GLY	-	expression tag	UNP Q89269
d	346	GLY	-	expression tag	UNP Q89269
d	347	GLY	-	expression tag	UNP Q89269
d	348	GLY	-	expression tag	UNP Q89269
d	349	SER	-	expression tag	UNP Q89269
d	350	GLY	-	expression tag	UNP Q89269
d	351	GLY	-	expression tag	UNP Q89269
d	352	GLY	-	expression tag	UNP Q89269
d	353	GLY	-	expression tag	UNP Q89269
d	354	SER	-	expression tag	UNP Q89269
d	355	GLY	-	expression tag	UNP Q89269
d	356	GLY	-	expression tag	UNP Q89269
d	357	GLY	-	expression tag	UNP Q89269
d	358	GLY	-	expression tag	UNP Q89269
d	359	SER	-	expression tag	UNP Q89269
d	360	MET	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
d	361	ASP	-	expression tag	UNP Q89269
d	362	TYR	-	expression tag	UNP Q89269
d	363	LYS	-	expression tag	UNP Q89269
d	364	ASP	-	expression tag	UNP Q89269
d	365	HIS	-	expression tag	UNP Q89269
d	366	ASP	-	expression tag	UNP Q89269
d	367	GLY	-	expression tag	UNP Q89269
d	368	ASP	-	expression tag	UNP Q89269
d	369	TYR	-	expression tag	UNP Q89269
d	370	LYS	-	expression tag	UNP Q89269
d	371	ASP	-	expression tag	UNP Q89269
d	372	HIS	-	expression tag	UNP Q89269
d	373	ASP	-	expression tag	UNP Q89269
d	374	ILE	-	expression tag	UNP Q89269
d	375	ASP	-	expression tag	UNP Q89269
d	376	TYR	-	expression tag	UNP Q89269
d	377	LYS	-	expression tag	UNP Q89269
d	378	ASP	-	expression tag	UNP Q89269
d	379	ASP	-	expression tag	UNP Q89269
d	380	ASP	-	expression tag	UNP Q89269
d	381	ASP	-	expression tag	UNP Q89269
d	382	LYS	-	expression tag	UNP Q89269
d	383	GLY	-	expression tag	UNP Q89269
d	384	SER	-	expression tag	UNP Q89269
d	385	GLU	-	expression tag	UNP Q89269
d	386	ASN	-	expression tag	UNP Q89269
d	387	LEU	-	expression tag	UNP Q89269
d	388	TYR	-	expression tag	UNP Q89269
d	389	PHE	-	expression tag	UNP Q89269
d	390	GLN	-	expression tag	UNP Q89269
d	391	SER	-	expression tag	UNP Q89269
d	392	HIS	-	expression tag	UNP Q89269
d	393	HIS	-	expression tag	UNP Q89269
d	394	HIS	-	expression tag	UNP Q89269
d	395	HIS	-	expression tag	UNP Q89269
d	396	HIS	-	expression tag	UNP Q89269
d	397	HIS	-	expression tag	UNP Q89269
e	1	GLU	-	expression tag	UNP Q89269
e	2	GLN	-	expression tag	UNP Q89269
e	3	ASN	-	expression tag	UNP Q89269
e	4	LYS	-	expression tag	UNP Q89269
e	5	GLU	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
e	6	ASN	-	expression tag	UNP Q89269
e	7	GLN	-	expression tag	UNP Q89269
e	8	ASN	-	expression tag	UNP Q89269
e	9	PRO	-	expression tag	UNP Q89269
e	10	ASN	-	expression tag	UNP Q89269
e	11	SER	-	expression tag	UNP Q89269
e	12	ASP	-	expression tag	UNP Q89269
e	13	ALA	-	expression tag	UNP Q89269
e	14	PRO	-	expression tag	UNP Q89269
e	15	VAL	-	expression tag	UNP Q89269
e	16	ILE	-	expression tag	UNP Q89269
e	17	ARG	-	expression tag	UNP Q89269
e	18	SER	-	expression tag	UNP Q89269
e	19	LYS	-	expression tag	UNP Q89269
e	20	THR	-	expression tag	UNP Q89269
e	21	SER	-	expression tag	UNP Q89269
e	22	ALA	-	expression tag	UNP Q89269
e	23	ARG	-	expression tag	UNP Q89269
e	24	TYR	-	expression tag	UNP Q89269
e	337	GLY	-	expression tag	UNP Q89269
e	338	SER	-	expression tag	UNP Q89269
e	339	LEU	-	expression tag	UNP Q89269
e	340	VAL	-	expression tag	UNP Q89269
e	341	PRO	-	expression tag	UNP Q89269
e	342	ARG	-	expression tag	UNP Q89269
e	343	GLY	-	expression tag	UNP Q89269
e	344	SER	-	expression tag	UNP Q89269
e	345	GLY	-	expression tag	UNP Q89269
e	346	GLY	-	expression tag	UNP Q89269
e	347	GLY	-	expression tag	UNP Q89269
e	348	GLY	-	expression tag	UNP Q89269
e	349	SER	-	expression tag	UNP Q89269
e	350	GLY	-	expression tag	UNP Q89269
e	351	GLY	-	expression tag	UNP Q89269
e	352	GLY	-	expression tag	UNP Q89269
e	353	GLY	-	expression tag	UNP Q89269
e	354	SER	-	expression tag	UNP Q89269
e	355	GLY	-	expression tag	UNP Q89269
e	356	GLY	-	expression tag	UNP Q89269
e	357	GLY	-	expression tag	UNP Q89269
e	358	GLY	-	expression tag	UNP Q89269
e	359	SER	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
e	360	MET	-	expression tag	UNP Q89269
e	361	ASP	-	expression tag	UNP Q89269
e	362	TYR	-	expression tag	UNP Q89269
e	363	LYS	-	expression tag	UNP Q89269
e	364	ASP	-	expression tag	UNP Q89269
e	365	HIS	-	expression tag	UNP Q89269
e	366	ASP	-	expression tag	UNP Q89269
e	367	GLY	-	expression tag	UNP Q89269
e	368	ASP	-	expression tag	UNP Q89269
e	369	TYR	-	expression tag	UNP Q89269
e	370	LYS	-	expression tag	UNP Q89269
e	371	ASP	-	expression tag	UNP Q89269
e	372	HIS	-	expression tag	UNP Q89269
e	373	ASP	-	expression tag	UNP Q89269
e	374	ILE	-	expression tag	UNP Q89269
e	375	ASP	-	expression tag	UNP Q89269
e	376	TYR	-	expression tag	UNP Q89269
e	377	LYS	-	expression tag	UNP Q89269
e	378	ASP	-	expression tag	UNP Q89269
e	379	ASP	-	expression tag	UNP Q89269
e	380	ASP	-	expression tag	UNP Q89269
e	381	ASP	-	expression tag	UNP Q89269
e	382	LYS	-	expression tag	UNP Q89269
e	383	GLY	-	expression tag	UNP Q89269
e	384	SER	-	expression tag	UNP Q89269
e	385	GLU	-	expression tag	UNP Q89269
e	386	ASN	-	expression tag	UNP Q89269
e	387	LEU	-	expression tag	UNP Q89269
e	388	TYR	-	expression tag	UNP Q89269
e	389	PHE	-	expression tag	UNP Q89269
e	390	GLN	-	expression tag	UNP Q89269
e	391	SER	-	expression tag	UNP Q89269
e	392	HIS	-	expression tag	UNP Q89269
e	393	HIS	-	expression tag	UNP Q89269
e	394	HIS	-	expression tag	UNP Q89269
e	395	HIS	-	expression tag	UNP Q89269
e	396	HIS	-	expression tag	UNP Q89269
e	397	HIS	-	expression tag	UNP Q89269
f	1	GLU	-	expression tag	UNP Q89269
f	2	GLN	-	expression tag	UNP Q89269
f	3	ASN	-	expression tag	UNP Q89269
f	4	LYS	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
f	5	GLU	-	expression tag	UNP Q89269
f	6	ASN	-	expression tag	UNP Q89269
f	7	GLN	-	expression tag	UNP Q89269
f	8	ASN	-	expression tag	UNP Q89269
f	9	PRO	-	expression tag	UNP Q89269
f	10	ASN	-	expression tag	UNP Q89269
f	11	SER	-	expression tag	UNP Q89269
f	12	ASP	-	expression tag	UNP Q89269
f	13	ALA	-	expression tag	UNP Q89269
f	14	PRO	-	expression tag	UNP Q89269
f	15	VAL	-	expression tag	UNP Q89269
f	16	ILE	-	expression tag	UNP Q89269
f	17	ARG	-	expression tag	UNP Q89269
f	18	SER	-	expression tag	UNP Q89269
f	19	LYS	-	expression tag	UNP Q89269
f	20	THR	-	expression tag	UNP Q89269
f	21	SER	-	expression tag	UNP Q89269
f	22	ALA	-	expression tag	UNP Q89269
f	23	ARG	-	expression tag	UNP Q89269
f	24	TYR	-	expression tag	UNP Q89269
f	337	GLY	-	expression tag	UNP Q89269
f	338	SER	-	expression tag	UNP Q89269
f	339	LEU	-	expression tag	UNP Q89269
f	340	VAL	-	expression tag	UNP Q89269
f	341	PRO	-	expression tag	UNP Q89269
f	342	ARG	-	expression tag	UNP Q89269
f	343	GLY	-	expression tag	UNP Q89269
f	344	SER	-	expression tag	UNP Q89269
f	345	GLY	-	expression tag	UNP Q89269
f	346	GLY	-	expression tag	UNP Q89269
f	347	GLY	-	expression tag	UNP Q89269
f	348	GLY	-	expression tag	UNP Q89269
f	349	SER	-	expression tag	UNP Q89269
f	350	GLY	-	expression tag	UNP Q89269
f	351	GLY	-	expression tag	UNP Q89269
f	352	GLY	-	expression tag	UNP Q89269
f	353	GLY	-	expression tag	UNP Q89269
f	354	SER	-	expression tag	UNP Q89269
f	355	GLY	-	expression tag	UNP Q89269
f	356	GLY	-	expression tag	UNP Q89269
f	357	GLY	-	expression tag	UNP Q89269
f	358	GLY	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
f	359	SER	-	expression tag	UNP Q89269
f	360	MET	-	expression tag	UNP Q89269
f	361	ASP	-	expression tag	UNP Q89269
f	362	TYR	-	expression tag	UNP Q89269
f	363	LYS	-	expression tag	UNP Q89269
f	364	ASP	-	expression tag	UNP Q89269
f	365	HIS	-	expression tag	UNP Q89269
f	366	ASP	-	expression tag	UNP Q89269
f	367	GLY	-	expression tag	UNP Q89269
f	368	ASP	-	expression tag	UNP Q89269
f	369	TYR	-	expression tag	UNP Q89269
f	370	LYS	-	expression tag	UNP Q89269
f	371	ASP	-	expression tag	UNP Q89269
f	372	HIS	-	expression tag	UNP Q89269
f	373	ASP	-	expression tag	UNP Q89269
f	374	ILE	-	expression tag	UNP Q89269
f	375	ASP	-	expression tag	UNP Q89269
f	376	TYR	-	expression tag	UNP Q89269
f	377	LYS	-	expression tag	UNP Q89269
f	378	ASP	-	expression tag	UNP Q89269
f	379	ASP	-	expression tag	UNP Q89269
f	380	ASP	-	expression tag	UNP Q89269
f	381	ASP	-	expression tag	UNP Q89269
f	382	LYS	-	expression tag	UNP Q89269
f	383	GLY	-	expression tag	UNP Q89269
f	384	SER	-	expression tag	UNP Q89269
f	385	GLU	-	expression tag	UNP Q89269
f	386	ASN	-	expression tag	UNP Q89269
f	387	LEU	-	expression tag	UNP Q89269
f	388	TYR	-	expression tag	UNP Q89269
f	389	PHE	-	expression tag	UNP Q89269
f	390	GLN	-	expression tag	UNP Q89269
f	391	SER	-	expression tag	UNP Q89269
f	392	HIS	-	expression tag	UNP Q89269
f	393	HIS	-	expression tag	UNP Q89269
f	394	HIS	-	expression tag	UNP Q89269
f	395	HIS	-	expression tag	UNP Q89269
f	396	HIS	-	expression tag	UNP Q89269
f	397	HIS	-	expression tag	UNP Q89269
g	1	GLU	-	expression tag	UNP Q89269
g	2	GLN	-	expression tag	UNP Q89269
g	3	ASN	-	expression tag	UNP Q89269

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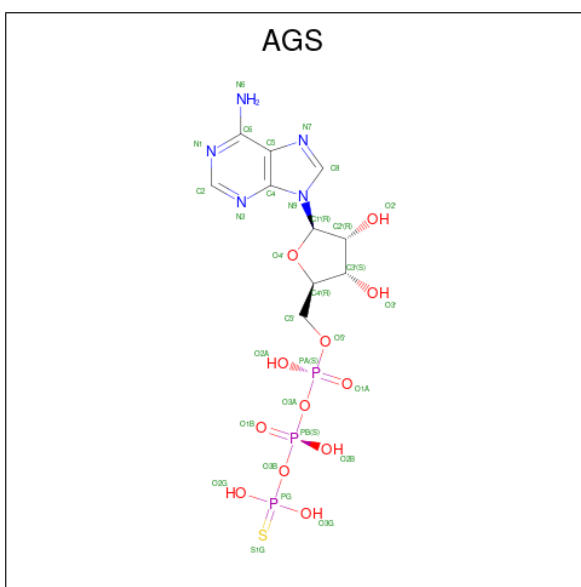
Chain	Residue	Modelled	Actual	Comment	Reference
g	4	LYS	-	expression tag	UNP Q89269
g	5	GLU	-	expression tag	UNP Q89269
g	6	ASN	-	expression tag	UNP Q89269
g	7	GLN	-	expression tag	UNP Q89269
g	8	ASN	-	expression tag	UNP Q89269
g	9	PRO	-	expression tag	UNP Q89269
g	10	ASN	-	expression tag	UNP Q89269
g	11	SER	-	expression tag	UNP Q89269
g	12	ASP	-	expression tag	UNP Q89269
g	13	ALA	-	expression tag	UNP Q89269
g	14	PRO	-	expression tag	UNP Q89269
g	15	VAL	-	expression tag	UNP Q89269
g	16	ILE	-	expression tag	UNP Q89269
g	17	ARG	-	expression tag	UNP Q89269
g	18	SER	-	expression tag	UNP Q89269
g	19	LYS	-	expression tag	UNP Q89269
g	20	THR	-	expression tag	UNP Q89269
g	21	SER	-	expression tag	UNP Q89269
g	22	ALA	-	expression tag	UNP Q89269
g	23	ARG	-	expression tag	UNP Q89269
g	24	TYR	-	expression tag	UNP Q89269
g	337	GLY	-	expression tag	UNP Q89269
g	338	SER	-	expression tag	UNP Q89269
g	339	LEU	-	expression tag	UNP Q89269
g	340	VAL	-	expression tag	UNP Q89269
g	341	PRO	-	expression tag	UNP Q89269
g	342	ARG	-	expression tag	UNP Q89269
g	343	GLY	-	expression tag	UNP Q89269
g	344	SER	-	expression tag	UNP Q89269
g	345	GLY	-	expression tag	UNP Q89269
g	346	GLY	-	expression tag	UNP Q89269
g	347	GLY	-	expression tag	UNP Q89269
g	348	GLY	-	expression tag	UNP Q89269
g	349	SER	-	expression tag	UNP Q89269
g	350	GLY	-	expression tag	UNP Q89269
g	351	GLY	-	expression tag	UNP Q89269
g	352	GLY	-	expression tag	UNP Q89269
g	353	GLY	-	expression tag	UNP Q89269
g	354	SER	-	expression tag	UNP Q89269
g	355	GLY	-	expression tag	UNP Q89269
g	356	GLY	-	expression tag	UNP Q89269
g	357	GLY	-	expression tag	UNP Q89269

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Chain	Residue	Modelled	Actual	Comment	Reference
g	358	GLY	-	expression tag	UNP Q89269
g	359	SER	-	expression tag	UNP Q89269
g	360	MET	-	expression tag	UNP Q89269
g	361	ASP	-	expression tag	UNP Q89269
g	362	TYR	-	expression tag	UNP Q89269
g	363	LYS	-	expression tag	UNP Q89269
g	364	ASP	-	expression tag	UNP Q89269
g	365	HIS	-	expression tag	UNP Q89269
g	366	ASP	-	expression tag	UNP Q89269
g	367	GLY	-	expression tag	UNP Q89269
g	368	ASP	-	expression tag	UNP Q89269
g	369	TYR	-	expression tag	UNP Q89269
g	370	LYS	-	expression tag	UNP Q89269
g	371	ASP	-	expression tag	UNP Q89269
g	372	HIS	-	expression tag	UNP Q89269
g	373	ASP	-	expression tag	UNP Q89269
g	374	ILE	-	expression tag	UNP Q89269
g	375	ASP	-	expression tag	UNP Q89269
g	376	TYR	-	expression tag	UNP Q89269
g	377	LYS	-	expression tag	UNP Q89269
g	378	ASP	-	expression tag	UNP Q89269
g	379	ASP	-	expression tag	UNP Q89269
g	380	ASP	-	expression tag	UNP Q89269
g	381	ASP	-	expression tag	UNP Q89269
g	382	LYS	-	expression tag	UNP Q89269
g	383	GLY	-	expression tag	UNP Q89269
g	384	SER	-	expression tag	UNP Q89269
g	385	GLU	-	expression tag	UNP Q89269
g	386	ASN	-	expression tag	UNP Q89269
g	387	LEU	-	expression tag	UNP Q89269
g	388	TYR	-	expression tag	UNP Q89269
g	389	PHE	-	expression tag	UNP Q89269
g	390	GLN	-	expression tag	UNP Q89269
g	391	SER	-	expression tag	UNP Q89269
g	392	HIS	-	expression tag	UNP Q89269
g	393	HIS	-	expression tag	UNP Q89269
g	394	HIS	-	expression tag	UNP Q89269
g	395	HIS	-	expression tag	UNP Q89269
g	396	HIS	-	expression tag	UNP Q89269
g	397	HIS	-	expression tag	UNP Q89269

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
3	a	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	b	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	a	1	Total Mg 1 1	0
4	b	1	Total Mg 1 1	0
4	c	1	Total Mg 1 1	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



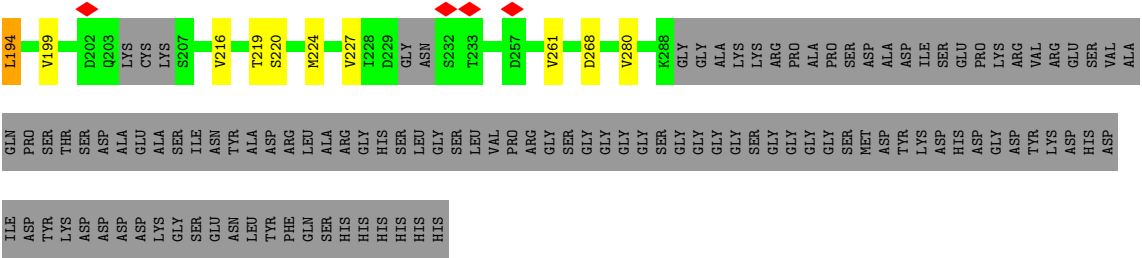
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	c	1	27	10	5	10	2	0

Chain c:  67% 30%

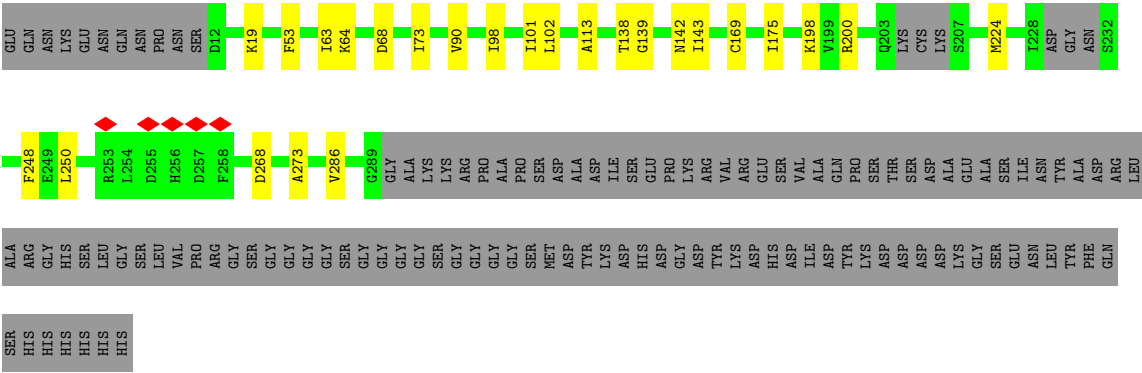
Chain d:  65% 5% 30%

Chain e: 61% 7% 31%

Chain f: 



● Molecule 2: Protein Rep40



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137594	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.99	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.453	Depositor
Minimum map value	-22.698	Depositor
Average map value	0.014	Depositor
Map value standard deviation	1.167	Depositor
Recommended contour level	4.87	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, ADP

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	H	0.17	0/642	0.87	0/986
2	a	0.13	0/2266	0.28	0/3068
2	b	0.13	0/2266	0.27	0/3068
2	c	0.12	0/2266	0.26	0/3068
2	d	0.12	0/2261	0.28	0/3060
2	e	0.12	0/2226	0.32	0/3015
2	f	0.13	0/2223	0.33	0/3010
2	g	0.12	0/2220	0.30	0/3005
All	All	0.13	0/16370	0.34	0/22280

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	574	0	313	0	0
2	a	2214	0	2180	7	0
2	b	2214	0	2180	10	0
2	c	2214	0	2181	7	0
2	d	2210	0	2177	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	e	2175	0	2136	23	0
2	f	2173	0	2133	27	0
2	g	2170	0	2135	21	0
3	a	31	0	12	0	0
3	b	31	0	12	1	0
4	a	1	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
5	c	27	0	12	0	0
All	All	16036	0	15471	106	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 3.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:187:VAL:HG21	2:f:227:VAL:HG13	1.66	0.76
2:f:224:MET:N	2:f:224:MET:HE2	2.01	0.76
2:g:139:GLY:O	2:g:143:ILE:HD12	1.89	0.73
2:e:182:MET:HA	2:e:182:MET:HE2	1.69	0.73
2:g:98:ILE:HD11	2:g:143:ILE:HG23	1.73	0.71
2:e:194:LEU:HB3	2:e:245:MET:HE1	1.74	0.69
2:d:224:MET:HE2	2:d:224:MET:C	2.20	0.66
2:c:37:THR:HG22	2:c:74:MET:HE1	1.80	0.64
2:d:224:MET:HE2	2:d:224:MET:O	1.97	0.64
2:f:151:VAL:HG21	2:f:174:VAL:HG12	1.80	0.63
2:g:248:PHE:CZ	2:g:286:VAL:HG21	2.34	0.61
2:e:210:GLN:C	2:e:211:ILE:HD12	2.28	0.59
2:d:146:ALA:HB2	2:d:261:VAL:HG23	1.85	0.58
2:f:169:CYS:SG	2:f:175:ILE:HD13	2.43	0.58
2:f:140:LYS:O	2:f:141:THR:HG22	2.04	0.58
2:b:186:VAL:HG12	2:b:186:VAL:O	2.03	0.58
2:d:182:MET:HE1	2:d:187:VAL:HG23	1.86	0.57
2:g:64:LYS:HE3	2:g:64:LYS:HA	1.86	0.57
2:b:171:ASP:O	2:b:171:ASP:OD2	2.23	0.56
2:f:193:ILE:HD12	2:f:199:VAL:HG11	1.86	0.55
2:f:129:THR:OG1	2:f:194:LEU:HD13	2.07	0.55
2:d:84:LEU:HD21	2:d:151:VAL:HG13	1.89	0.54
2:a:218:VAL:HG11	2:a:224:MET:HE2	1.88	0.54
2:a:113:ALA:HB1	2:a:273:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:77:THR:O	2:e:77:THR:HG22	2.08	0.54
2:e:177:TRP:CD1	2:e:218:VAL:HG13	2.43	0.53
2:f:68:ASP:OD2	2:f:68:ASP:C	2.52	0.53
2:e:68:ASP:OD2	2:e:68:ASP:C	2.52	0.53
2:g:68:ASP:OD1	2:g:68:ASP:C	2.52	0.52
3:b:1000:AGS:H8	3:b:1000:AGS:C5'	2.40	0.52
2:f:224:MET:HE2	2:f:224:MET:H	1.73	0.52
2:f:90:VAL:HG21	2:f:268:ASP:CG	2.35	0.52
2:c:68:ASP:C	2:c:68:ASP:OD1	2.52	0.51
2:e:131:TRP:O	2:e:132:LEU:HD13	2.11	0.49
2:e:117:LEU:HD21	2:e:274:LYS:HE3	1.94	0.49
2:g:143:ILE:HD12	2:g:143:ILE:H	1.76	0.49
2:e:100:LYS:O	2:e:104:LEU:HD13	2.13	0.49
2:g:102:LEU:HD23	2:g:250:LEU:HD11	1.95	0.49
2:f:146:ALA:HB2	2:f:261:VAL:HG23	1.95	0.48
2:f:116:PHE:HA	2:f:119:TRP:HD1	1.78	0.48
2:e:121:THR:O	2:e:121:THR:HG22	2.13	0.48
2:f:51:ILE:HD11	2:g:73:ILE:HD11	1.94	0.48
2:g:98:ILE:CD1	2:g:143:ILE:HG23	2.42	0.48
2:a:194:LEU:HD23	2:a:245:MET:HE3	1.96	0.47
2:b:211:ILE:HG23	2:b:211:ILE:O	2.14	0.47
2:d:151:VAL:HG21	2:d:174:VAL:HG12	1.97	0.47
2:d:102:LEU:HD23	2:d:112:ALA:HB3	1.96	0.47
2:g:98:ILE:HD13	2:g:101:ILE:HD11	1.97	0.46
2:a:252:ARG:HA	2:a:252:ARG:NH1	2.30	0.46
2:e:193:ILE:HG23	2:e:211:ILE:HG21	1.97	0.46
2:f:70:ALA:O	2:f:74:MET:HE2	2.16	0.46
2:d:170:VAL:O	2:d:171:ASP:OD1	2.33	0.46
2:f:186:VAL:HG22	2:f:186:VAL:O	2.15	0.46
2:b:113:ALA:HB1	2:b:273:ALA:HB2	1.98	0.46
2:a:252:ARG:HA	2:a:252:ARG:HH11	1.81	0.45
2:a:79:THR:HG22	2:a:82:ASP:OD2	2.16	0.45
2:e:37:THR:HG22	2:e:74:MET:HE1	1.99	0.45
2:e:117:LEU:HD21	2:e:274:LYS:CE	2.47	0.45
2:g:113:ALA:HB1	2:g:273:ALA:HB2	1.99	0.45
2:b:228:ILE:O	2:b:228:ILE:HD12	2.16	0.45
2:f:187:VAL:HG12	2:f:187:VAL:O	2.18	0.44
2:g:198:LYS:HB3	2:g:200:ARG:HH12	1.82	0.44
2:g:53:PHE:HB3	2:g:63:ILE:HD11	1.98	0.44
2:e:119:TRP:CZ2	2:e:217:ILE:HG23	2.53	0.44
2:e:131:TRP:CD2	2:e:224:MET:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:90:VAL:HG21	2:g:268:ASP:HB3	1.98	0.44
2:g:169:CYS:SG	2:g:175:ILE:HD12	2.58	0.44
2:e:157:VAL:HG21	2:e:177:TRP:HE3	1.83	0.44
2:c:113:ALA:HB1	2:c:273:ALA:HB2	2.00	0.43
2:d:145:GLU:OE2	2:d:145:GLU:HA	2.18	0.43
2:e:127:ARG:HA	2:e:244:ARG:C	2.44	0.43
2:f:51:ILE:HD11	2:g:73:ILE:CD1	2.48	0.43
2:b:22:ALA:O	2:b:26:GLU:HG2	2.19	0.43
2:f:143:ILE:HA	2:f:261:VAL:HG21	2.00	0.43
2:f:64:LYS:HB3	2:f:64:LYS:NZ	2.33	0.43
2:e:154:TYR:CD2	2:e:154:TYR:C	2.97	0.43
2:f:187:VAL:CG2	2:f:227:VAL:HG13	2.43	0.43
2:f:220:SER:OG	2:f:224:MET:HE1	2.19	0.43
2:f:182:MET:O	2:f:182:MET:SD	2.77	0.43
2:g:248:PHE:CE2	2:g:286:VAL:HG21	2.52	0.43
2:f:21:SER:O	2:f:25:MET:HG3	2.19	0.42
2:g:138:THR:O	2:g:138:THR:HG22	2.19	0.42
2:g:139:GLY:O	2:g:142:ASN:HB3	2.19	0.42
2:d:99:TYR:C	2:d:99:TYR:CD1	2.97	0.42
2:c:77:THR:HG23	2:c:78:LYS:HG2	2.00	0.42
2:e:131:TRP:HZ3	2:e:218:VAL:HG11	1.84	0.42
2:e:187:VAL:HG22	2:e:188:GLU:H	1.84	0.42
2:b:186:VAL:O	2:b:186:VAL:CG1	2.68	0.42
2:c:138:THR:O	2:c:138:THR:HG22	2.20	0.42
2:b:171:ASP:OD2	2:b:171:ASP:C	2.63	0.41
2:f:124:PHE:CZ	2:f:280:VAL:HG11	2.55	0.41
2:a:175:ILE:HB	2:a:216:VAL:HG22	2.01	0.41
2:c:90:VAL:HG21	2:c:268:ASP:O	2.21	0.41
2:e:177:TRP:CD1	2:e:177:TRP:C	2.99	0.41
2:f:175:ILE:HG13	2:f:216:VAL:HG13	2.02	0.41
2:f:182:MET:SD	2:f:182:MET:C	3.03	0.41
2:b:90:VAL:O	2:b:90:VAL:HG23	2.21	0.41
2:b:256:HIS:ND1	2:b:256:HIS:C	2.78	0.41
2:c:17:ARG:HH11	2:c:17:ARG:HG2	1.84	0.41
2:f:132:LEU:HD23	2:f:219:THR:HG22	2.01	0.41
2:g:19:LYS:HD3	2:g:19:LYS:C	2.46	0.41
2:e:187:VAL:HG22	2:e:188:GLU:N	2.35	0.40
2:d:80:ALA:N	2:d:81:PRO:HD2	2.36	0.40
2:d:203:GLN:OE1	2:d:207:SER:O	2.40	0.40
2:e:199:VAL:HG22	2:e:200:ARG:N	2.36	0.40
2:g:224:MET:HE3	2:g:224:MET:HA	2.02	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	a	276/397 (70%)	271 (98%)	5 (2%)	0	100	100
2	b	276/397 (70%)	268 (97%)	8 (3%)	0	100	100
2	c	276/397 (70%)	271 (98%)	5 (2%)	0	100	100
2	d	273/397 (69%)	267 (98%)	6 (2%)	0	100	100
2	e	269/397 (68%)	257 (96%)	12 (4%)	0	100	100
2	f	266/397 (67%)	256 (96%)	10 (4%)	0	100	100
2	g	266/397 (67%)	259 (97%)	7 (3%)	0	100	100
All	All	1902/2779 (68%)	1849 (97%)	53 (3%)	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	a	240/333 (72%)	240 (100%)	0	100	100
2	b	240/333 (72%)	239 (100%)	1 (0%)	84	94
2	c	240/333 (72%)	240 (100%)	0	100	100
2	d	240/333 (72%)	240 (100%)	0	100	100
2	e	235/333 (71%)	232 (99%)	3 (1%)	61	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	f	235/333 (71%)	233 (99%)	2 (1%)	70	88
2	g	235/333 (71%)	235 (100%)	0	100	100
All	All	1665/2331 (71%)	1659 (100%)	6 (0%)	81	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	256	HIS
2	e	37	THR
2	e	102	LEU
2	e	245	MET
2	f	67	LEU
2	f	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	96	ASN
2	a	210	GLN
2	b	167	ASN
2	d	149	HIS
2	d	282	HIS
2	f	44	GLN
2	g	167	ASN
2	g	210	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
3	AGS	a	1000	4	32,33,33	0.50	1 (3%)	45,52,52	1.08	3 (6%)
3	AGS	b	1000	4	32,33,33	0.73	1 (3%)	45,52,52	0.72	1 (2%)
5	ADP	c	1000	4	28,29,29	1.37	4 (14%)	43,45,45	1.90	10 (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
3	AGS	a	1000	4	-	6/21/38/38	0/3/3/3
3	AGS	b	1000	4	-	5/21/38/38	0/3/3/3
5	ADP	c	1000	4	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	1000	ADP	C5-C4	4.43	1.47	1.39
5	c	1000	ADP	C5-C6	2.55	1.48	1.41
5	c	1000	ADP	C5-N7	-2.46	1.34	1.39
5	c	1000	ADP	C8-N7	2.23	1.36	1.31
3	b	1000	AGS	PB-O3B	-2.09	1.57	1.59
3	a	1000	AGS	PG-S1G	2.04	1.95	1.90

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	1000	ADP	C5-C4-N3	-5.84	118.68	126.72
5	c	1000	ADP	N3-C4-N9	4.82	135.36	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1000	AGS	C2'-C1'-N9	4.11	123.51	113.30
5	c	1000	ADP	C2-N3-C4	3.85	121.23	111.83
3	b	1000	AGS	PB-O3B-PG	-3.74	119.49	133.17
5	c	1000	ADP	N3-C2-N1	-3.70	122.98	128.58
3	a	1000	AGS	O4'-C1'-N9	3.62	115.04	108.09
3	a	1000	AGS	PB-O3B-PG	-3.57	120.10	133.17
5	c	1000	ADP	C4-C5-N7	-3.29	106.82	110.58
5	c	1000	ADP	C4-N9-C8	3.04	108.93	105.74
5	c	1000	ADP	C5-N7-C8	2.68	107.66	103.45
5	c	1000	ADP	C3'-C2'-C1'	2.52	106.23	101.46
5	c	1000	ADP	N9-C8-N7	-2.33	110.63	113.94
5	c	1000	ADP	C2-N1-C6	2.02	122.06	118.73

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	a	1000	AGS	O4'-C4'-C5'-O5'
3	b	1000	AGS	C5'-O5'-PA-O2A
3	b	1000	AGS	C5'-O5'-PA-O3A
5	c	1000	ADP	C5'-O5'-PA-O1A
5	c	1000	ADP	C5'-O5'-PA-O2A
5	c	1000	ADP	C5'-O5'-PA-O3A
3	a	1000	AGS	C3'-C4'-C5'-O5'
3	b	1000	AGS	O4'-C4'-C5'-O5'
3	b	1000	AGS	C3'-C4'-C5'-O5'
3	b	1000	AGS	PA-O3A-PB-O2B
3	a	1000	AGS	C4'-C5'-O5'-PA
3	a	1000	AGS	PA-O3A-PB-O1B
3	a	1000	AGS	PA-O3A-PB-O2B
3	a	1000	AGS	PG-O3B-PB-O1B

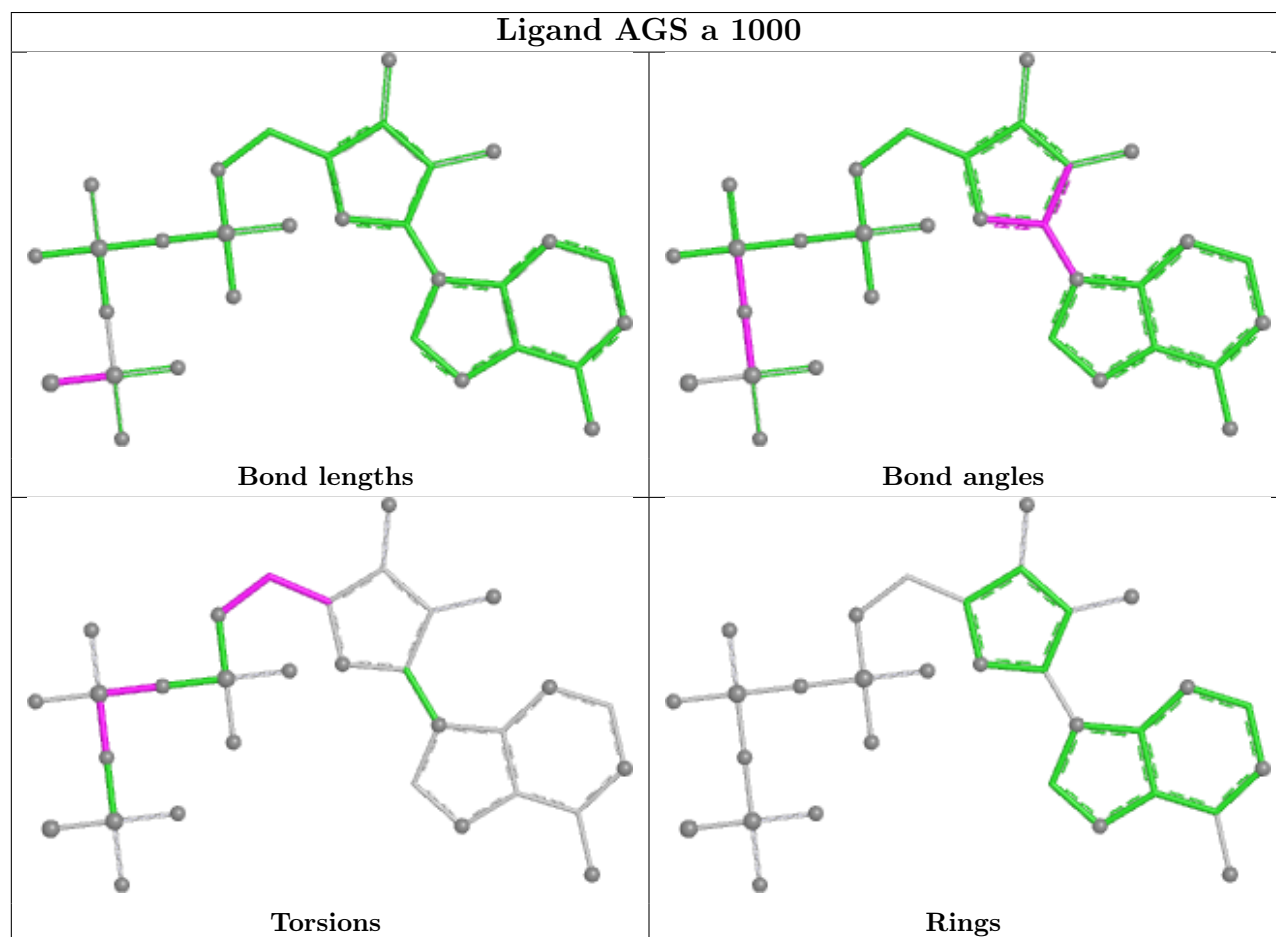
There are no ring outliers.

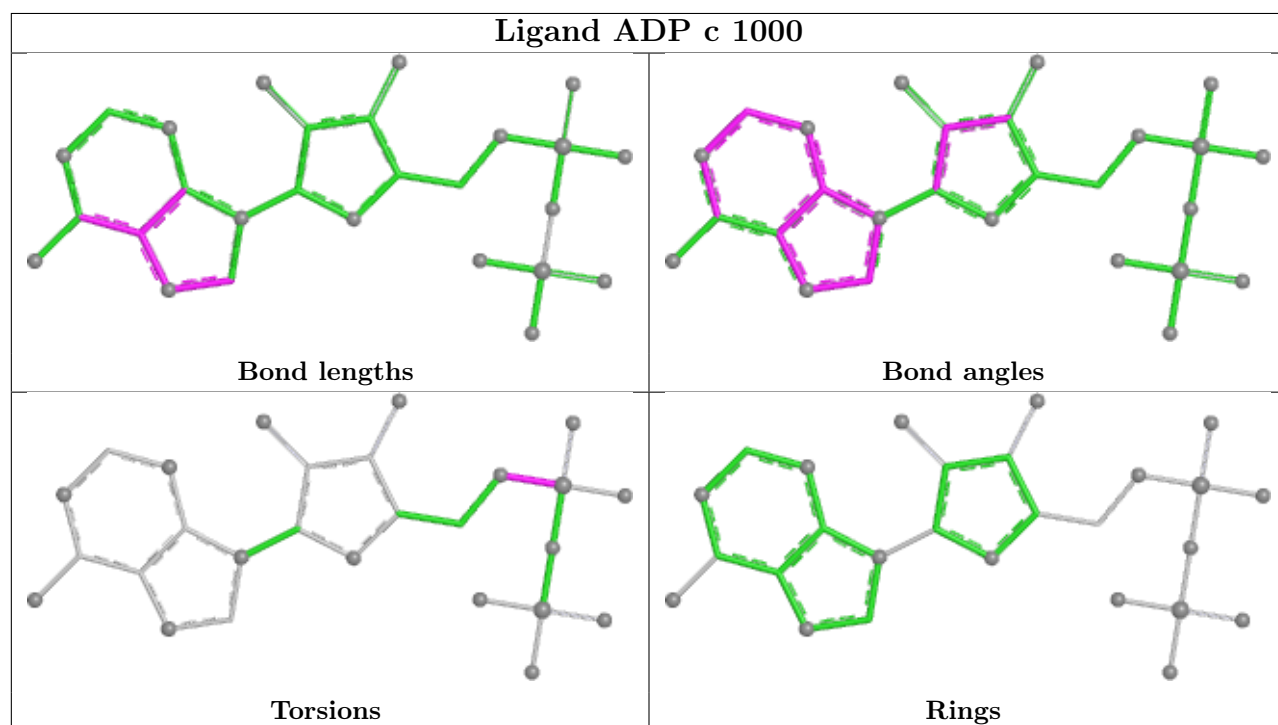
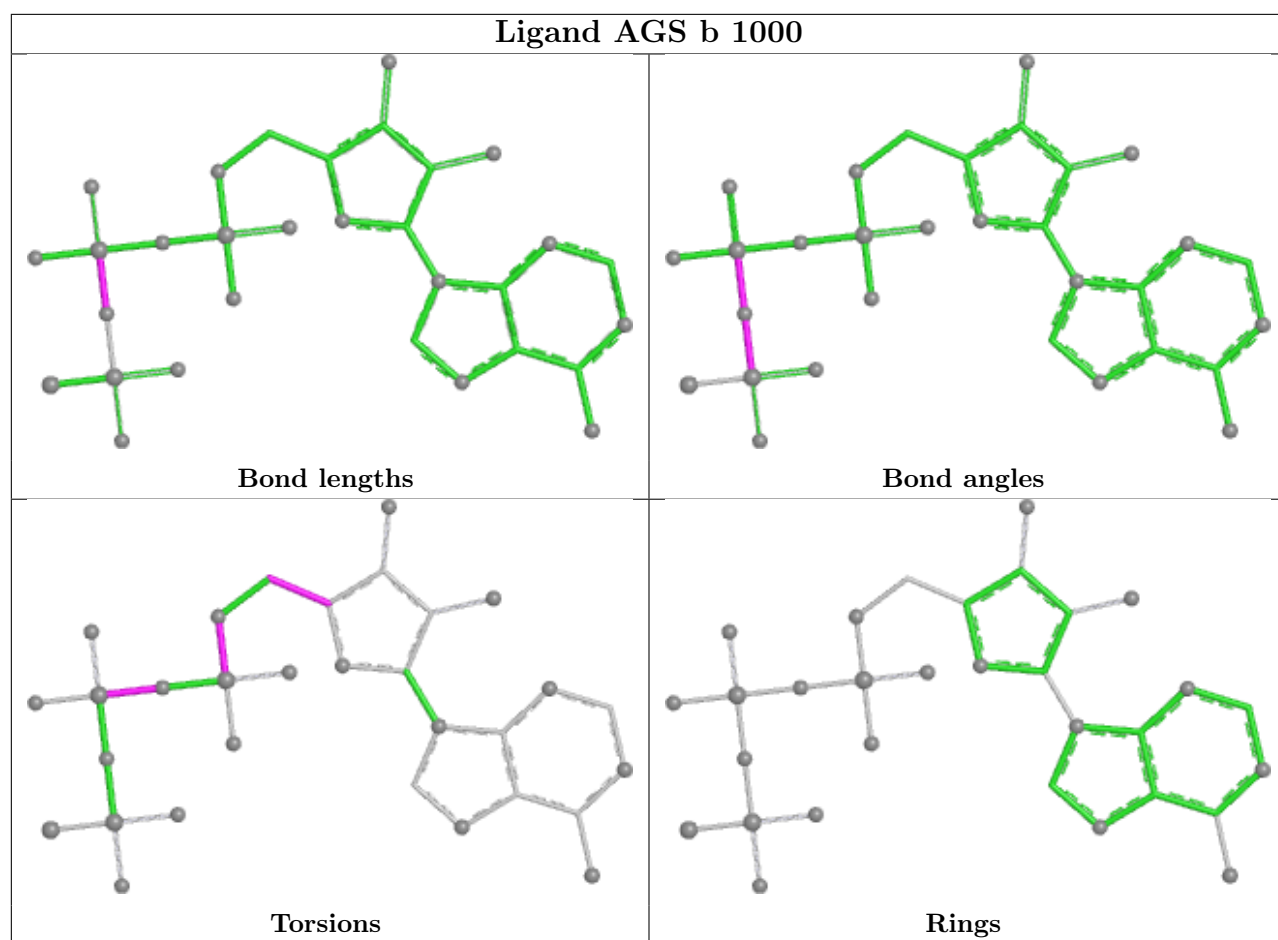
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	b	1000	AGS	1	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

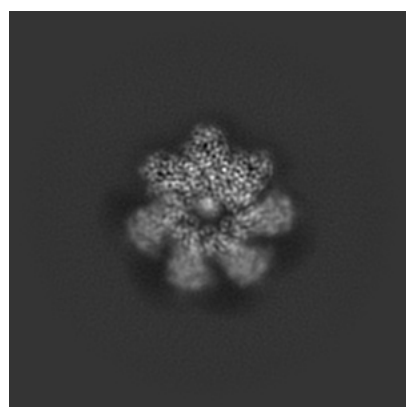
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54184. These allow visual inspection of the internal detail of the map and identification of artifacts.

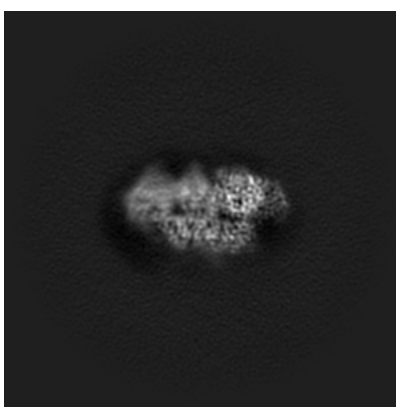
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

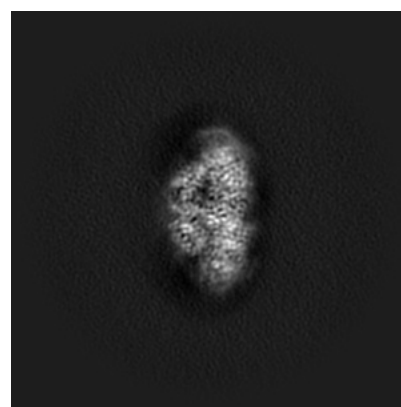
6.1.1 Primary map



X



Y

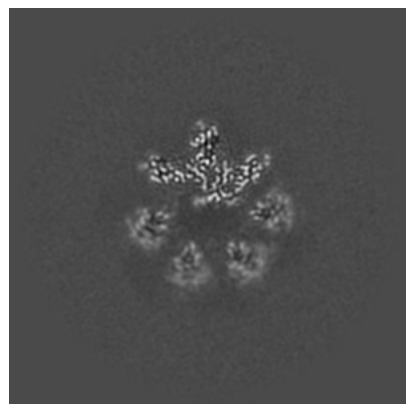


Z

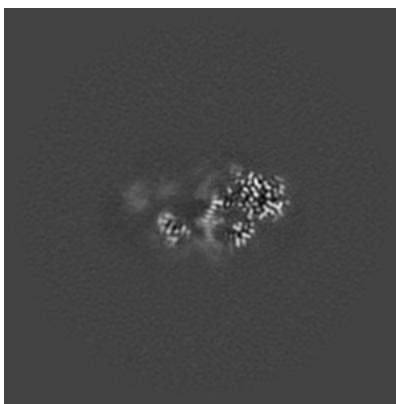
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

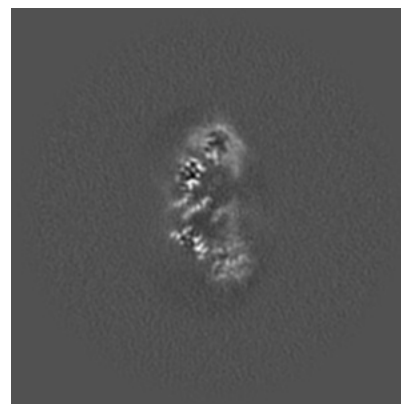
6.2.1 Primary map



X Index: 180



Y Index: 180

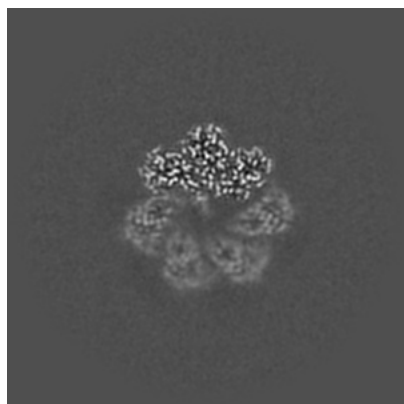


Z Index: 180

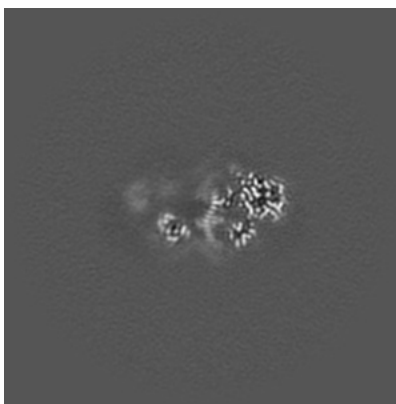
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

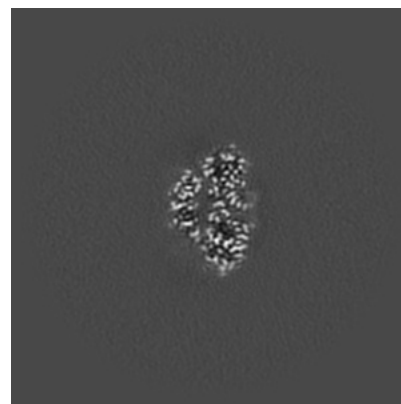
6.3.1 Primary map



X Index: 192



Y Index: 179

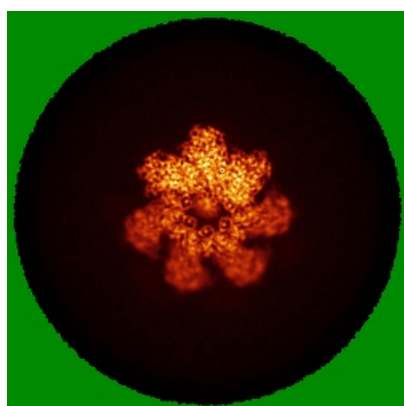


Z Index: 210

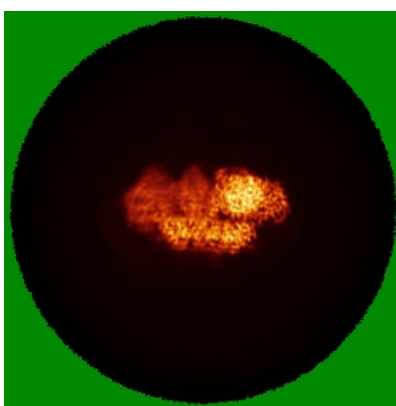
The images above show the largest variance slices of the map in three orthogonal directions.

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

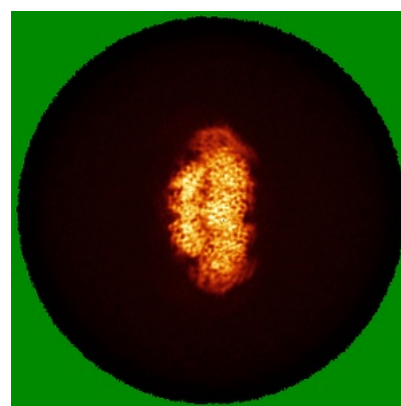
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.87. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

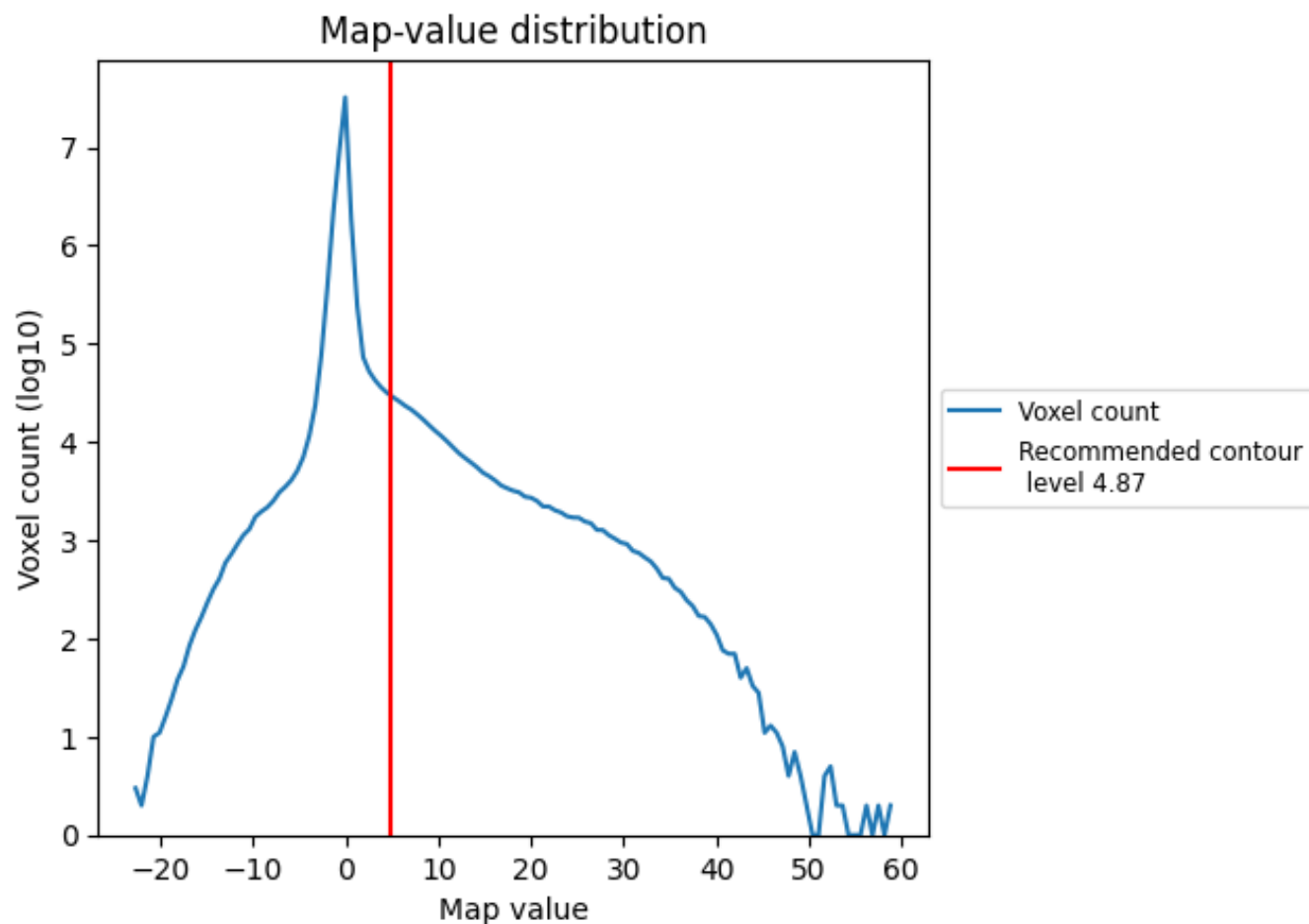
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

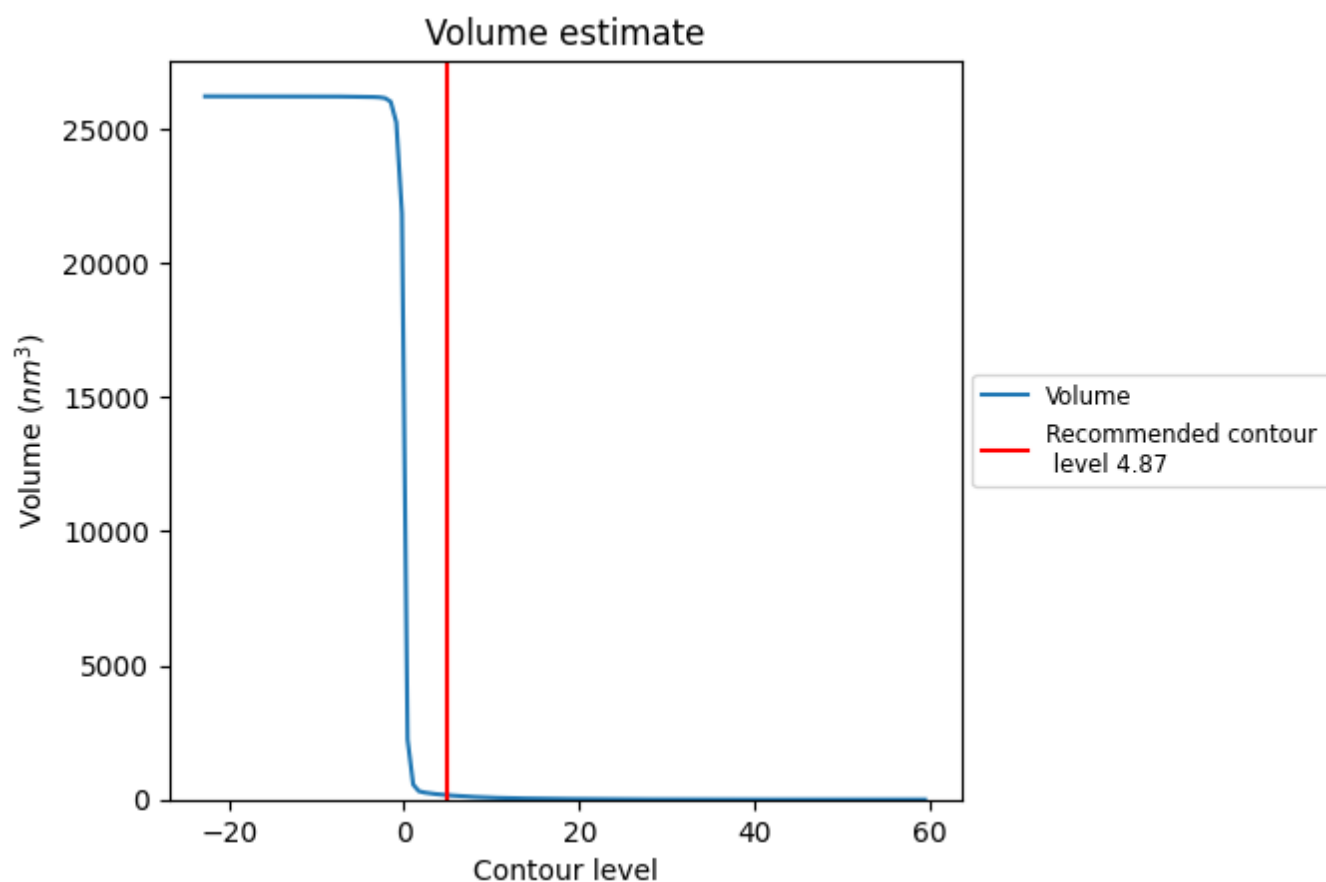
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

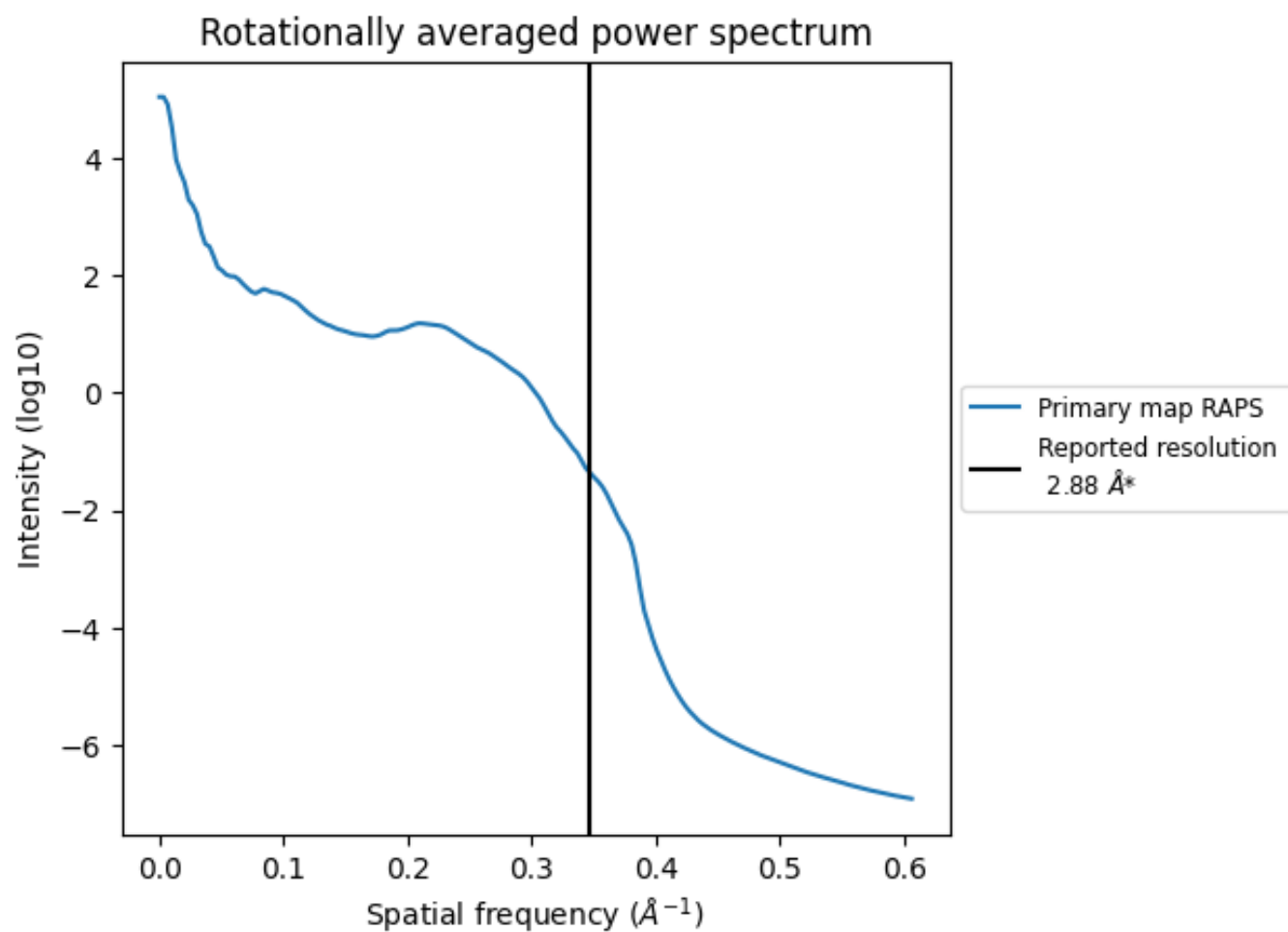
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm^3 ; this corresponds to an approximate mass of 150 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.347 Å⁻¹

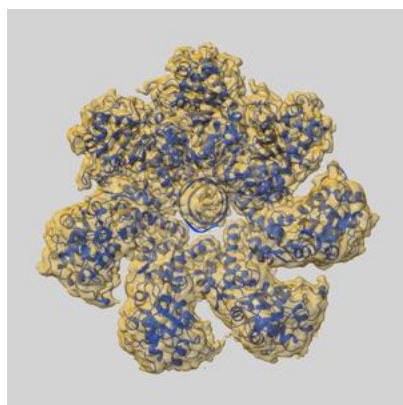
8 Fourier-Shell correlation

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

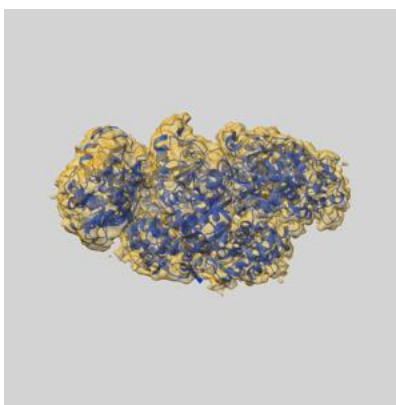
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54184 and PDB model 9RQT. Per-residue inclusion information can be found in section [3](#) on page [21](#).

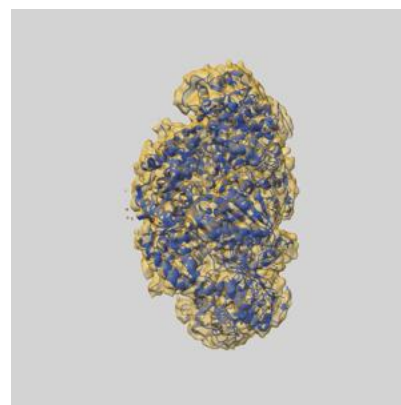
9.1 Map-model overlay [i](#)



X



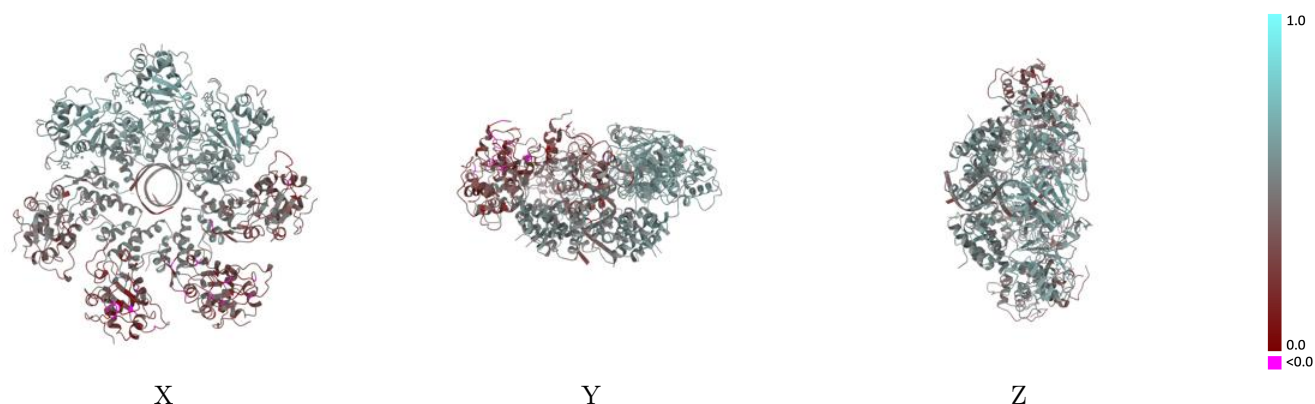
Y



Z

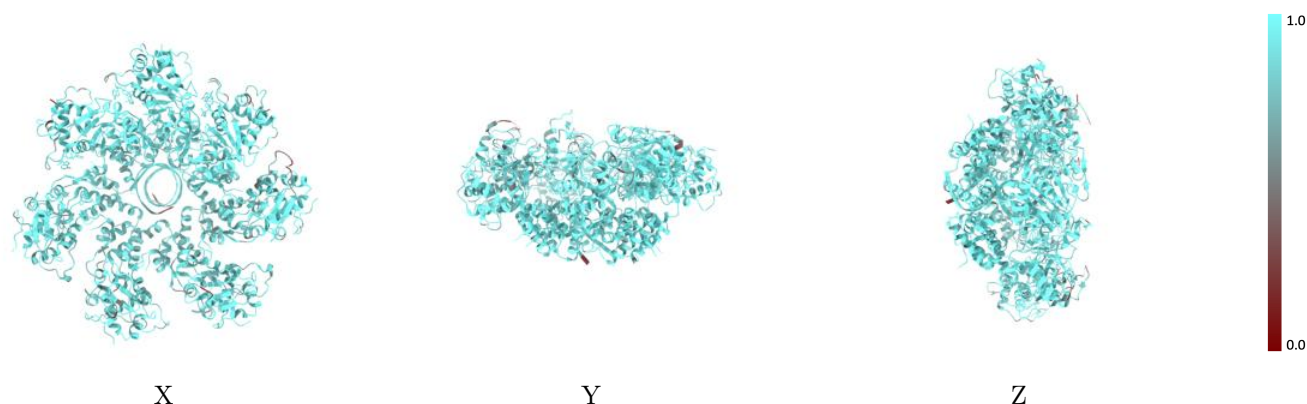
The images above show the 3D surface view of the map at the recommended contour level 4.87 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



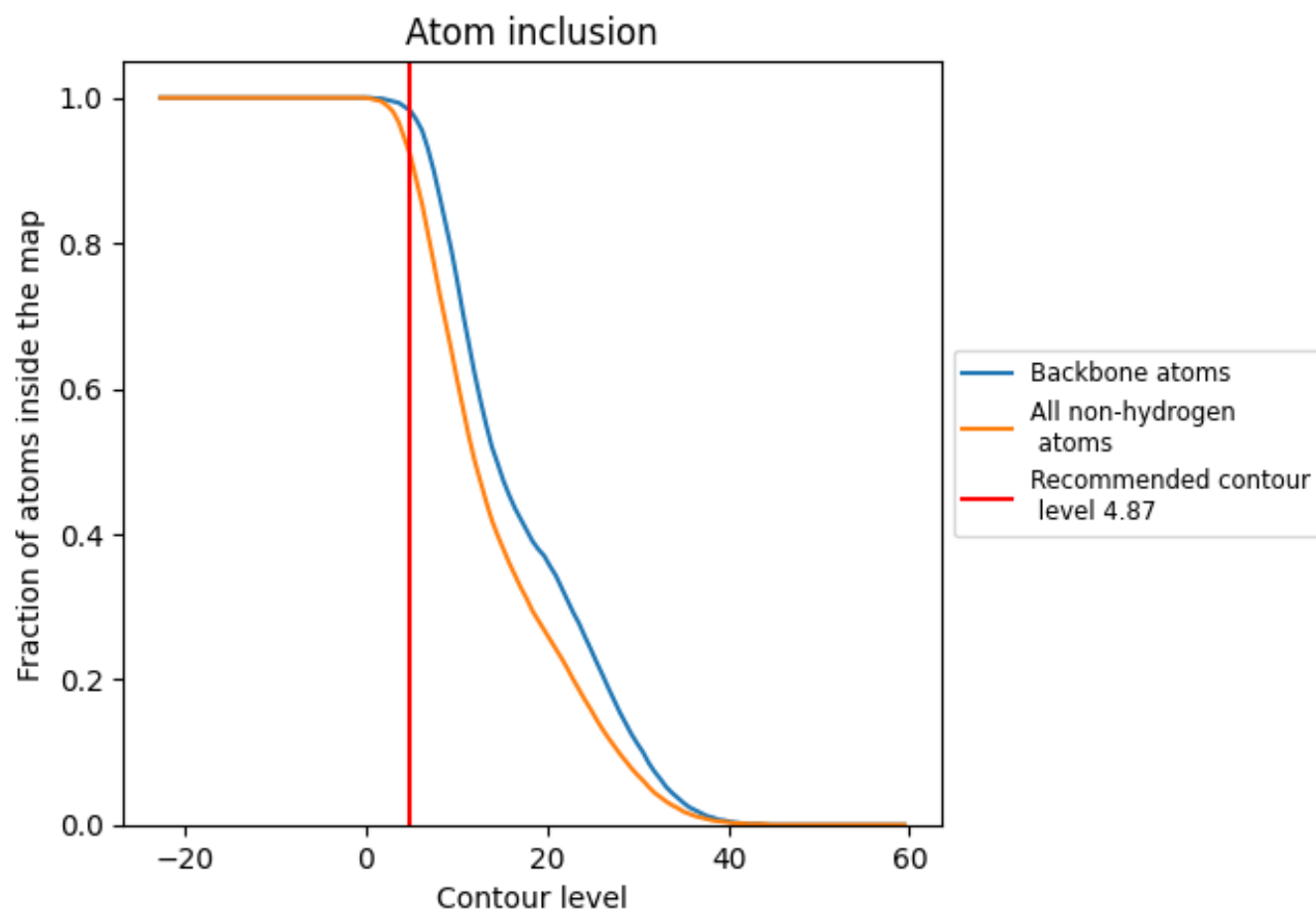
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.87).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (4.87) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9210</div>	<div><div></div>0.4610</div>
H	<div><div></div>0.8690</div>	<div><div></div>0.4000</div>
a	<div><div></div>0.9510</div>	<div><div></div>0.5600</div>
b	<div><div></div>0.9610</div>	<div><div></div>0.5750</div>
c	<div><div></div>0.9520</div>	<div><div></div>0.5630</div>
d	<div><div></div>0.9060</div>	<div><div></div>0.4330</div>
e	<div><div></div>0.8930</div>	<div><div></div>0.3450</div>
f	<div><div></div>0.8990</div>	<div><div></div>0.3580</div>
g	<div><div></div>0.8930</div>	<div><div></div>0.3980</div>

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