Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 12:41 PM JST

PDB ID	:	7CM7
EMDB ID	:	EMD-30403
Title	:	NAD+-bound Sarm1 E642A in the self-inhibited state
Authors	:	Zhang, Z.; Jiang, Y.
Deposited on	:	2020-07-25
Resolution	:	2.60 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 (1)) were used in the production of this report:

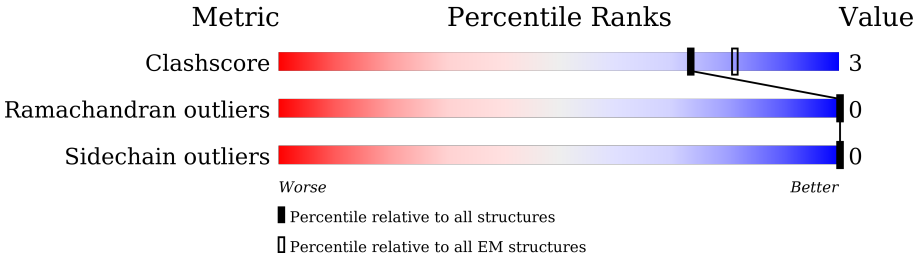
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	733	13% 76% 8% 15%
1	B	733	13% 76% 8% 15%
1	C	733	13% 76% 8% 15%
1	D	733	13% 76% 8% 15%
1	E	733	13% 76% 8% 15%
1	F	733	13% 76% 8% 15%
1	G	733	13% 76% 8% 15%
1	H	733	13% 77% 8% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 39216 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NAD(+) hydrolase SARM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	620	4858	3072	874	889	23	0	0
1	B	620	4858	3072	874	889	23	0	0
1	C	620	4858	3072	874	889	23	0	0
1	D	620	4858	3072	874	889	23	0	0
1	E	620	4858	3072	874	889	23	0	0
1	F	620	4858	3072	874	889	23	0	0
1	G	620	4858	3072	874	889	23	0	0
1	H	620	4858	3072	874	889	23	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	ALA	GLU	engineered mutation	UNP Q6SZW1
A	725	SER	-	expression tag	UNP Q6SZW1
A	726	ASN	-	expression tag	UNP Q6SZW1
A	727	SER	-	expression tag	UNP Q6SZW1
A	728	LEU	-	expression tag	UNP Q6SZW1
A	729	GLU	-	expression tag	UNP Q6SZW1
A	730	VAL	-	expression tag	UNP Q6SZW1
A	731	LEU	-	expression tag	UNP Q6SZW1
A	732	PHE	-	expression tag	UNP Q6SZW1
A	733	GLN	-	expression tag	UNP Q6SZW1
B	642	ALA	GLU	engineered mutation	UNP Q6SZW1
B	725	SER	-	expression tag	UNP Q6SZW1
B	726	ASN	-	expression tag	UNP Q6SZW1
B	727	SER	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	728	LEU	-	expression tag	UNP Q6SZW1
B	729	GLU	-	expression tag	UNP Q6SZW1
B	730	VAL	-	expression tag	UNP Q6SZW1
B	731	LEU	-	expression tag	UNP Q6SZW1
B	732	PHE	-	expression tag	UNP Q6SZW1
B	733	GLN	-	expression tag	UNP Q6SZW1
C	642	ALA	GLU	engineered mutation	UNP Q6SZW1
C	725	SER	-	expression tag	UNP Q6SZW1
C	726	ASN	-	expression tag	UNP Q6SZW1
C	727	SER	-	expression tag	UNP Q6SZW1
C	728	LEU	-	expression tag	UNP Q6SZW1
C	729	GLU	-	expression tag	UNP Q6SZW1
C	730	VAL	-	expression tag	UNP Q6SZW1
C	731	LEU	-	expression tag	UNP Q6SZW1
C	732	PHE	-	expression tag	UNP Q6SZW1
C	733	GLN	-	expression tag	UNP Q6SZW1
D	642	ALA	GLU	engineered mutation	UNP Q6SZW1
D	725	SER	-	expression tag	UNP Q6SZW1
D	726	ASN	-	expression tag	UNP Q6SZW1
D	727	SER	-	expression tag	UNP Q6SZW1
D	728	LEU	-	expression tag	UNP Q6SZW1
D	729	GLU	-	expression tag	UNP Q6SZW1
D	730	VAL	-	expression tag	UNP Q6SZW1
D	731	LEU	-	expression tag	UNP Q6SZW1
D	732	PHE	-	expression tag	UNP Q6SZW1
D	733	GLN	-	expression tag	UNP Q6SZW1
E	642	ALA	GLU	engineered mutation	UNP Q6SZW1
E	725	SER	-	expression tag	UNP Q6SZW1
E	726	ASN	-	expression tag	UNP Q6SZW1
E	727	SER	-	expression tag	UNP Q6SZW1
E	728	LEU	-	expression tag	UNP Q6SZW1
E	729	GLU	-	expression tag	UNP Q6SZW1
E	730	VAL	-	expression tag	UNP Q6SZW1
E	731	LEU	-	expression tag	UNP Q6SZW1
E	732	PHE	-	expression tag	UNP Q6SZW1
E	733	GLN	-	expression tag	UNP Q6SZW1
F	642	ALA	GLU	engineered mutation	UNP Q6SZW1
F	725	SER	-	expression tag	UNP Q6SZW1
F	726	ASN	-	expression tag	UNP Q6SZW1
F	727	SER	-	expression tag	UNP Q6SZW1
F	728	LEU	-	expression tag	UNP Q6SZW1
F	729	GLU	-	expression tag	UNP Q6SZW1

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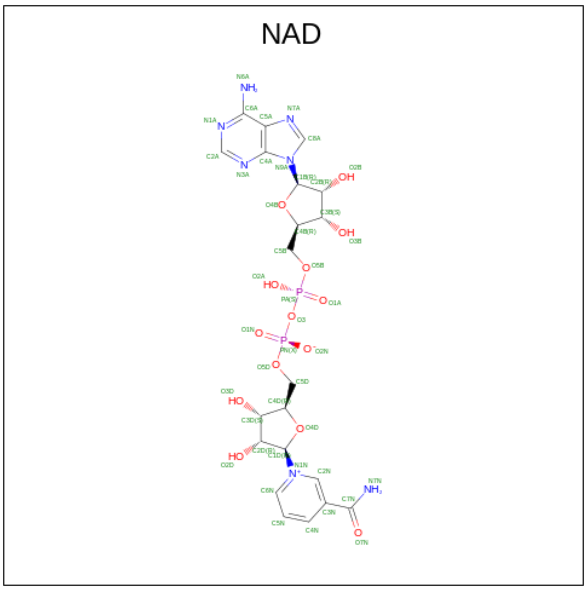
Chain	Residue	Modelled	Actual	Comment	Reference
F	730	VAL	-	expression tag	UNP Q6SZW1
F	731	LEU	-	expression tag	UNP Q6SZW1
F	732	PHE	-	expression tag	UNP Q6SZW1
F	733	GLN	-	expression tag	UNP Q6SZW1
G	642	ALA	GLU	engineered mutation	UNP Q6SZW1
G	725	SER	-	expression tag	UNP Q6SZW1
G	726	ASN	-	expression tag	UNP Q6SZW1
G	727	SER	-	expression tag	UNP Q6SZW1
G	728	LEU	-	expression tag	UNP Q6SZW1
G	729	GLU	-	expression tag	UNP Q6SZW1
G	730	VAL	-	expression tag	UNP Q6SZW1
G	731	LEU	-	expression tag	UNP Q6SZW1
G	732	PHE	-	expression tag	UNP Q6SZW1
G	733	GLN	-	expression tag	UNP Q6SZW1
H	642	ALA	GLU	engineered mutation	UNP Q6SZW1
H	725	SER	-	expression tag	UNP Q6SZW1
H	726	ASN	-	expression tag	UNP Q6SZW1
H	727	SER	-	expression tag	UNP Q6SZW1
H	728	LEU	-	expression tag	UNP Q6SZW1
H	729	GLU	-	expression tag	UNP Q6SZW1
H	730	VAL	-	expression tag	UNP Q6SZW1
H	731	LEU	-	expression tag	UNP Q6SZW1
H	732	PHE	-	expression tag	UNP Q6SZW1
H	733	GLN	-	expression tag	UNP Q6SZW1

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



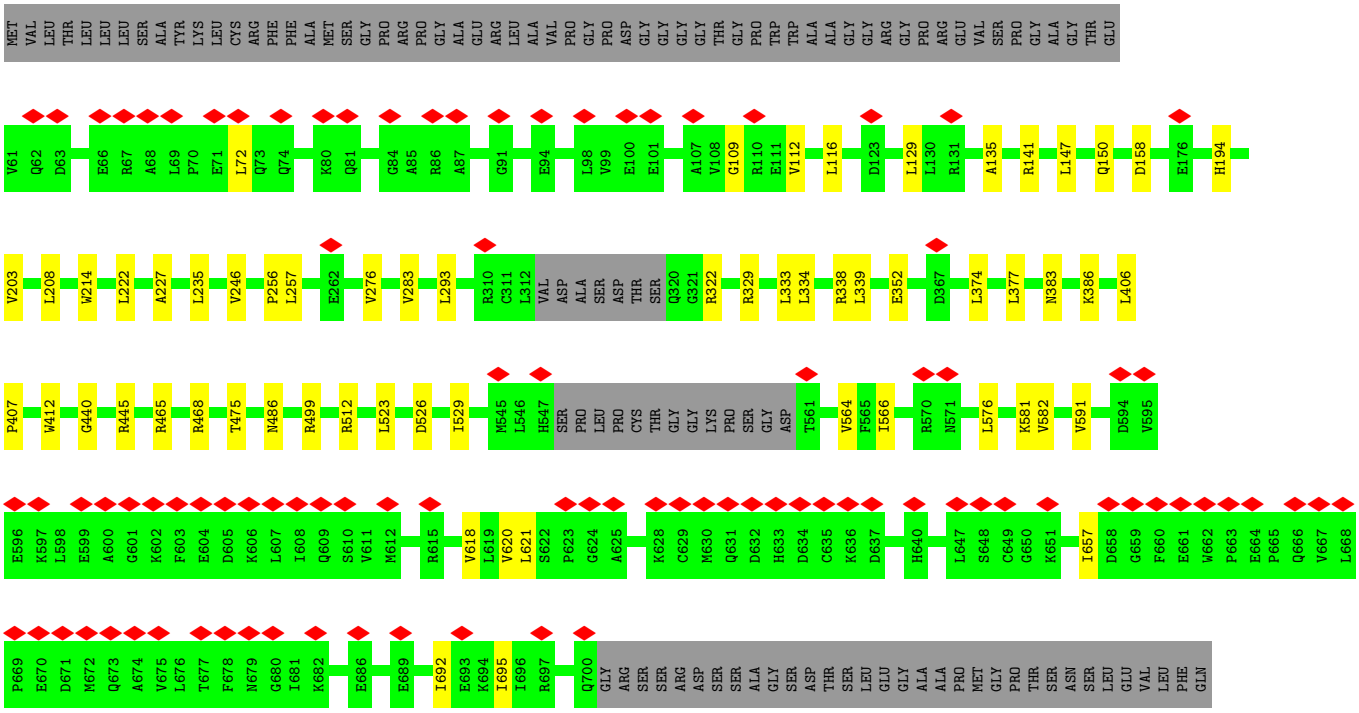
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	44	21	7	14	2	0
2	B	1	44	21	7	14	2	0
2	C	1	44	21	7	14	2	0
2	D	1	44	21	7	14	2	0
2	E	1	44	21	7	14	2	0
2	F	1	44	21	7	14	2	0
2	G	1	44	21	7	14	2	0
2	H	1	44	21	7	14	2	0

3 Residue-property plots (i)

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

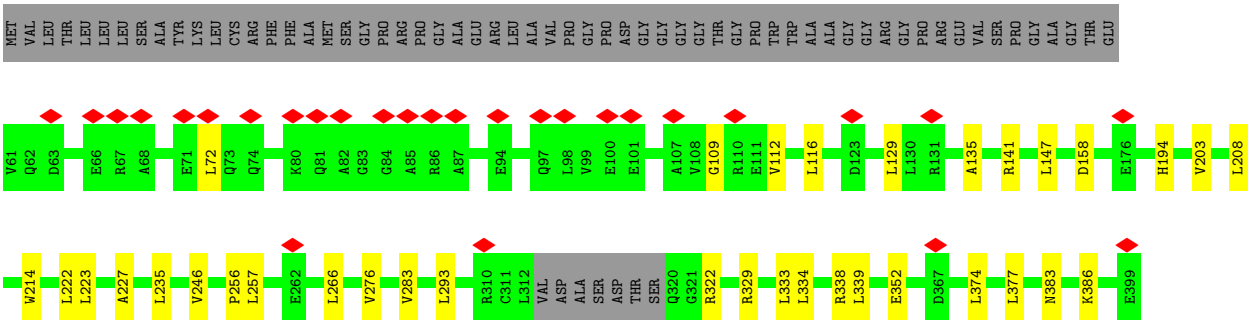
- Molecule 1: NAD(+) hydrolase SARM1

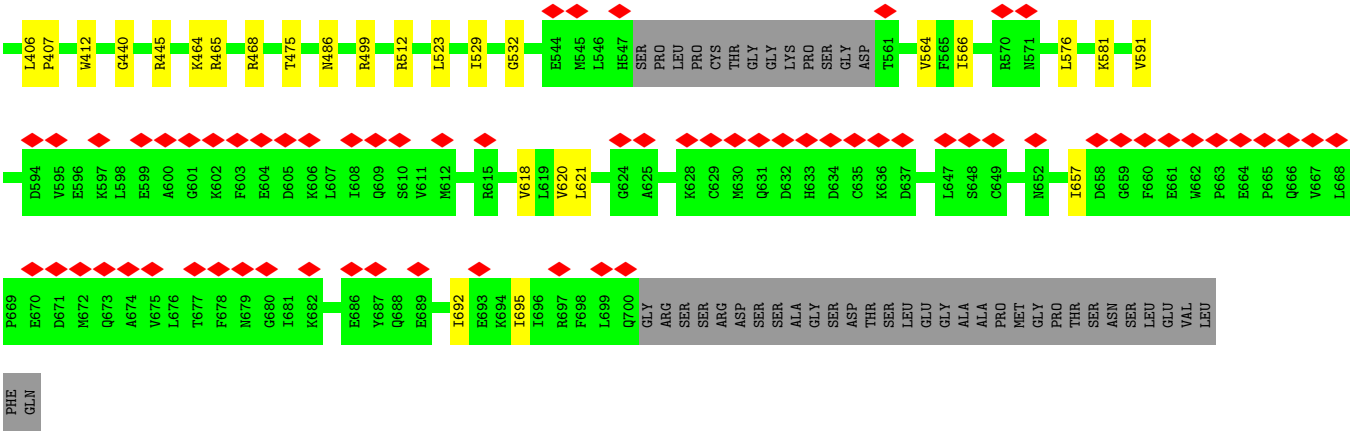
Chain A:



- Molecule 1: NAD(+) hydrolase SARM1

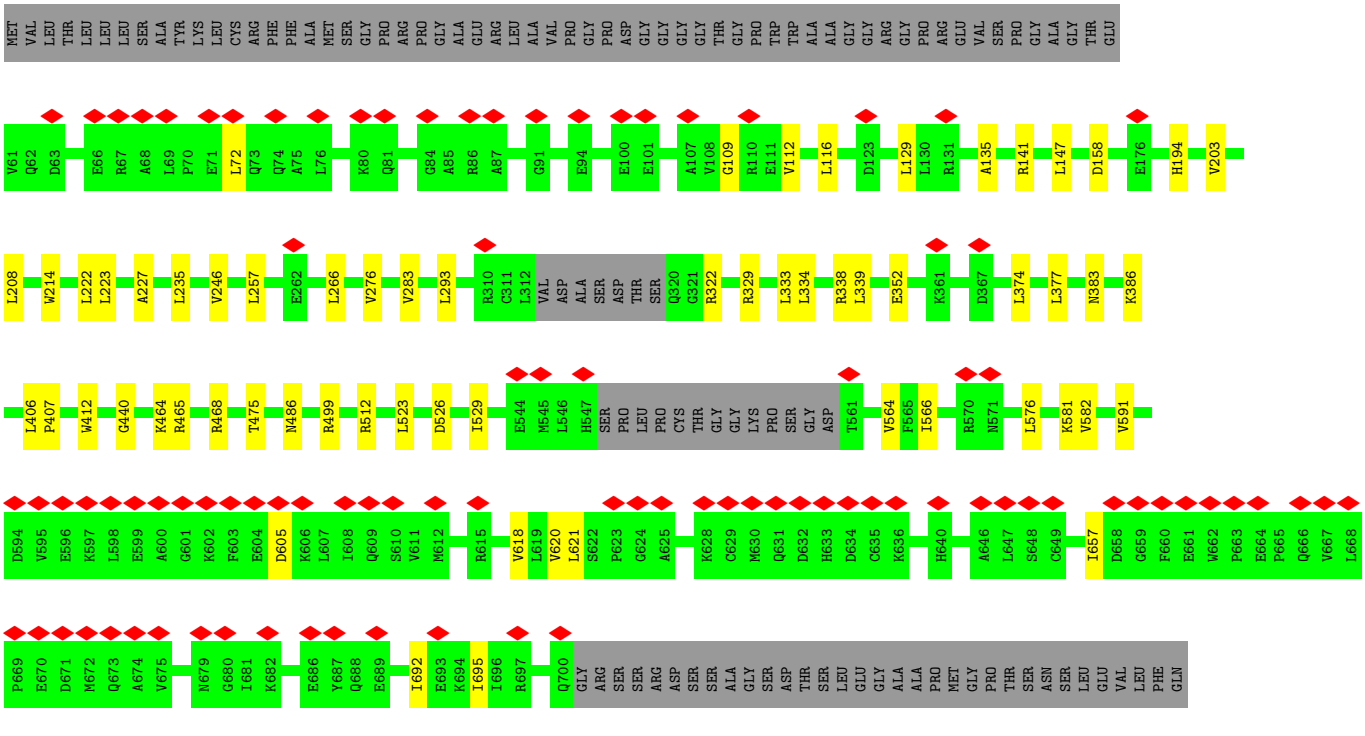
Chain B:





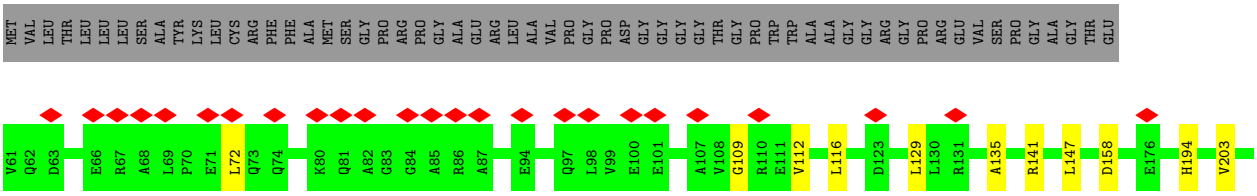
- Molecule 1: NAD(+) hydrolase SARM1

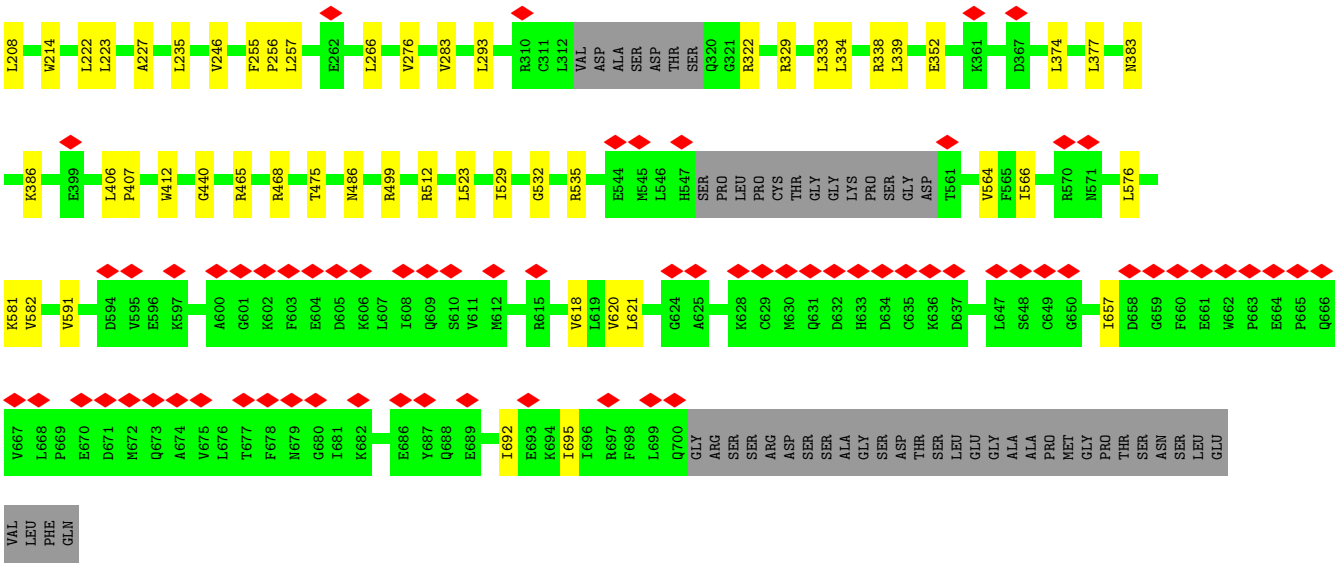
Chain C:



- Molecule 1: NAD(+) hydrolase SARM1

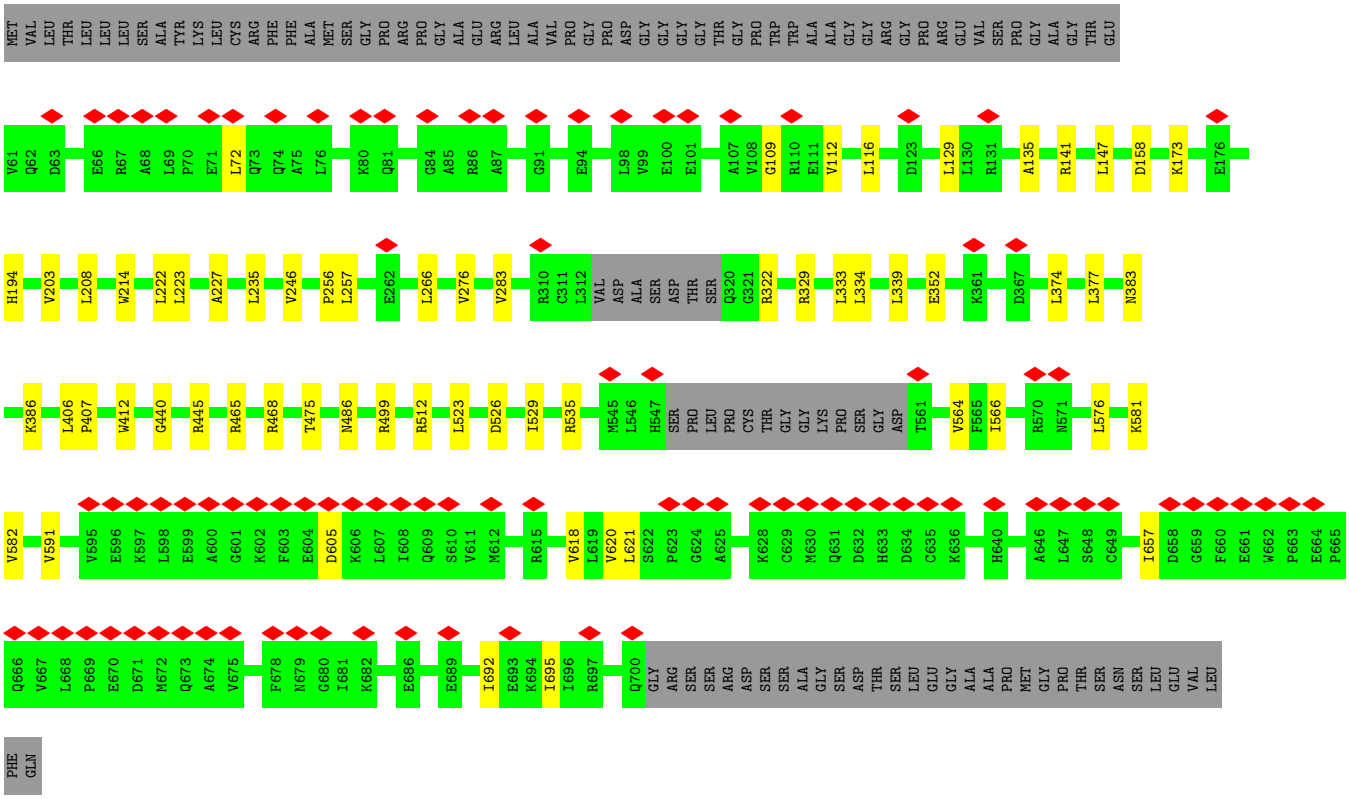
Chain D:





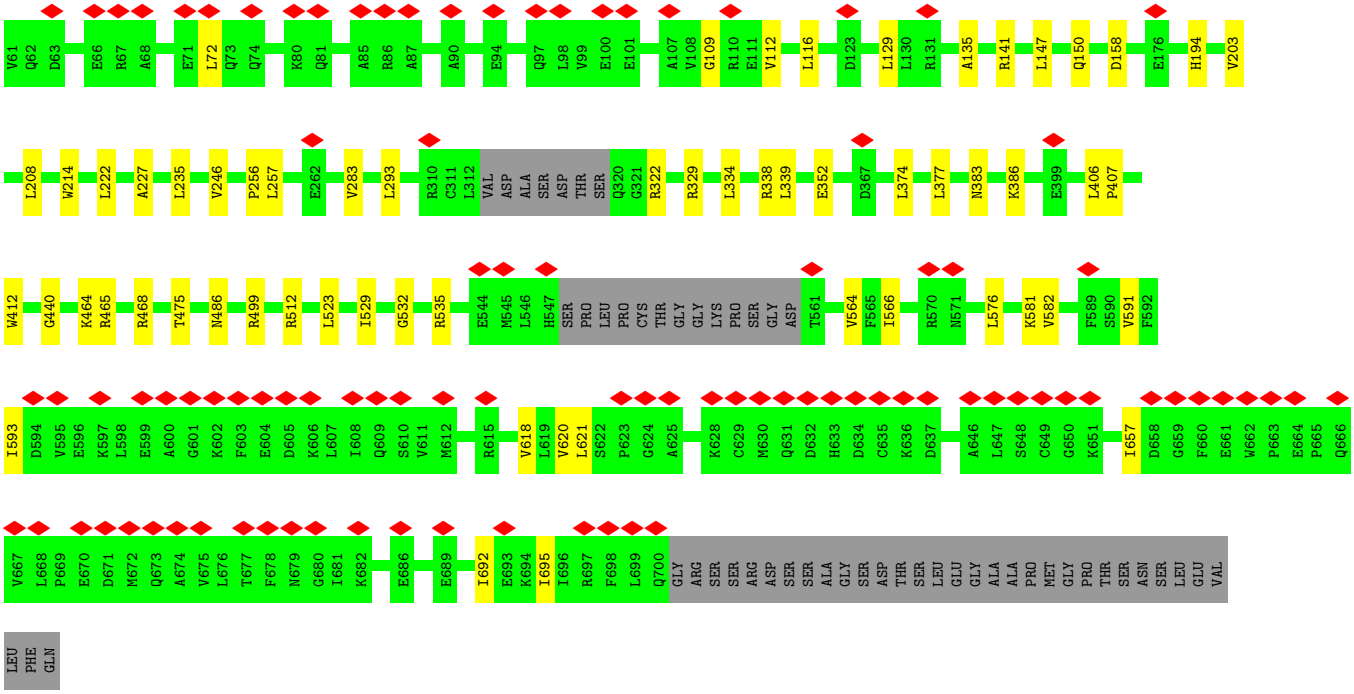
- Molecule 1: NAD(+) hydrolase SARM1

Chain E:



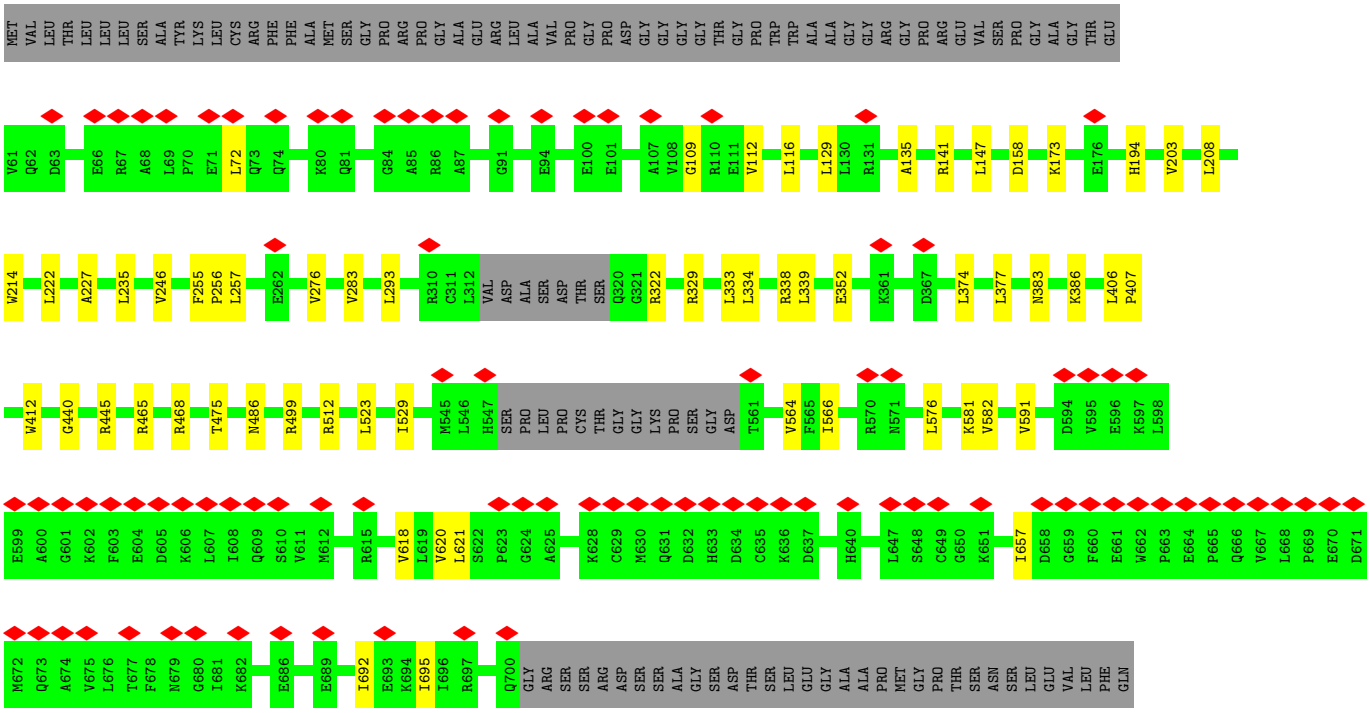
- Molecule 1: NAD(+) hydrolase SARM1

Chain F:



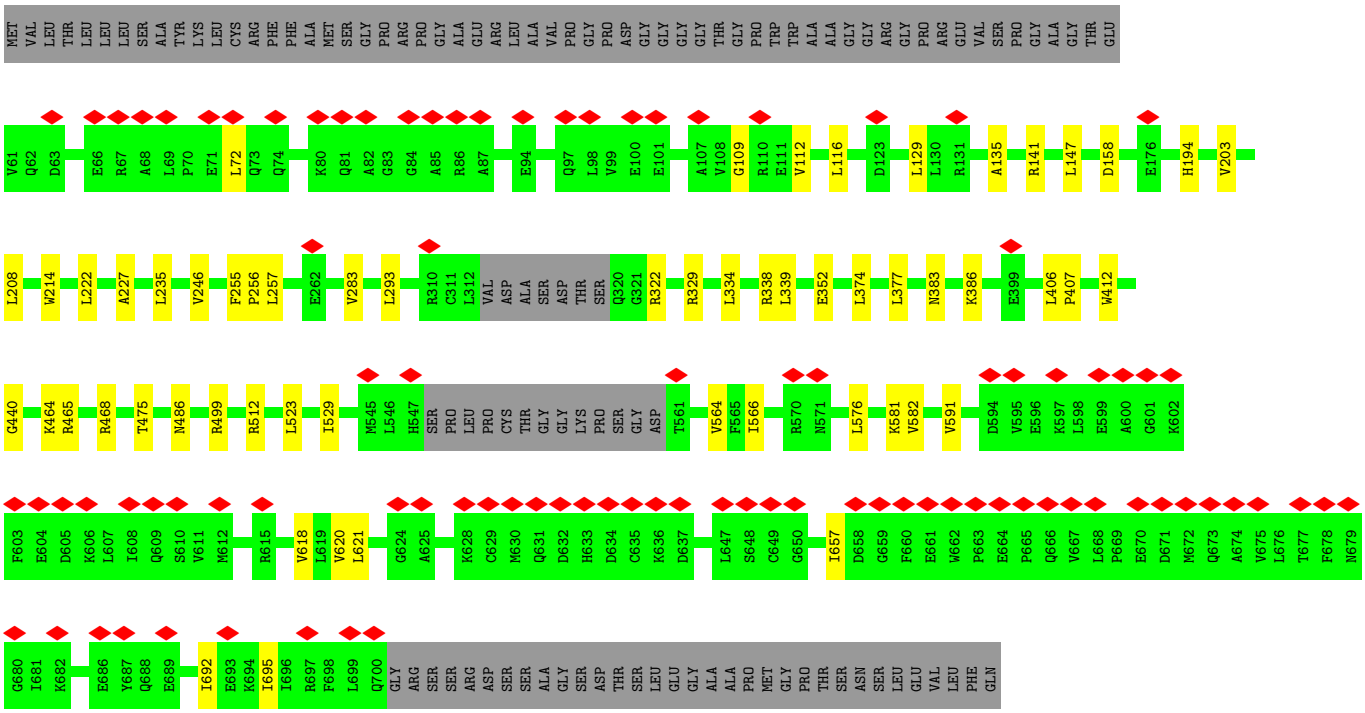
- Molecule 1: NAD(+) hydrolase SARM1

Chain G:



- Molecule 1: NAD(+) hydrolase SARM1

Chain H:


MET VAL LEU THR LEU LEU LEU LEU SER ALA TYR LYS LEU CYS ARG PHE PHE ALA MET SER GLY PRO ARG PRO GLY ALA GLU ARG LEU ALA VAL PRO GLY PRO ASP GLY GLY GLY GLY THR GLY PRO TRP TRP ALA ALA GLY GLY ARG GLY PRO ARG GLU VAL SER PRO GLY ALA GLY THR GLU
V61 Q62 D63 E66 R67 A68 L69 P70 E71 L72 Q73 Q74 K80 Q81 A82 G83 G84 A85 R86 A87 E94 Q97 L98 V99 E100 E101 A107 V108 G109 R110 E111 V112 L116 D123 L129 L130 R131 A135 R141 L147 D158 E176 H194 V203
L208 W214 L222 A227 L235 V246 F255 P256 L257 E262 V283 L293 R310 C311 L312 VAL ASP ALA SER ASP THR SER Q320 G321 R322 R329 L334 R338 L339 E352 L374 L377 N383 K386 E399 L406 P407 W412
G440 K464 R465 R468 T475 N486 R499 R512 L523 I529 M545 L546 H547 SER PRO LEU PRO CYS THR GLY GLY LYS PRO SER GLY ASP T561 V564 F565 I566 R570 N571 L576 K581 V582 V591 D594 V595 E596 K597 L598 E599 A600 G601 K602
F603 E604 D605 K606 L607 I608 Q609 S610 V611 M612 R615 V618 L619 V620 L621 G624 A625 K628 C629 M630 Q631 D632 H633 D634 C635 K636 D637 L647 S648 C649 G650 I657 D658 G659 F660 E661 W662 P663 E664 P665 Q666 V667 L668 P669 E670 D671 M672 Q673 A674 V675 L676 T677 F678 N679
G680 I681 K682 E686 Y687 Q688 E689 I692 E693 K694 I695 I696 R697 F698 L699 Q700 GLY ARG SER SER ARG ASP SER SER ALA GLY SER ASP THR SER LEU GLU GLY ALA ALA PRO MET GLY PRO THR SER ASN SER LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C8	Depositor
Number of particles used	137909	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.128	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	405.12, 405.12, 405.12	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	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: NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.25	0/4938	0.47	0/6673
1	B	0.25	0/4938	0.47	0/6673
1	C	0.25	0/4938	0.47	0/6673
1	D	0.25	0/4938	0.47	0/6673
1	E	0.25	0/4938	0.47	0/6673
1	F	0.25	0/4938	0.47	0/6673
1	G	0.25	0/4938	0.47	0/6673
1	H	0.25	0/4938	0.47	0/6673
All	All	0.25	0/39504	0.47	0/53384

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	A	4858	0	4948	34	0
1	B	4858	0	4948	34	0
1	C	4858	0	4948	35	0
1	D	4858	0	4948	35	0
1	E	4858	0	4948	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4858	0	4948	35	0
1	G	4858	0	4948	35	0
1	H	4858	0	4948	32	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	1	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
All	All	39216	0	39792	257	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 (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:VAL:HG21	1:D:256:PRO:HD3	1.81	0.61
1:D:475:THR:O	1:D:499:ARG:NH1	2.40	0.55
1:E:475:THR:O	1:E:499:ARG:NH1	2.40	0.54
1:B:475:THR:O	1:B:499:ARG:NH1	2.40	0.54
1:A:475:THR:O	1:A:499:ARG:NH1	2.40	0.54
1:H:475:THR:O	1:H:499:ARG:NH1	2.40	0.54
1:F:475:THR:O	1:F:499:ARG:NH1	2.40	0.54
1:B:214:TRP:HB3	1:B:222:LEU:HD21	1.90	0.54
1:C:214:TRP:HB3	1:C:222:LEU:HD21	1.90	0.54
1:C:475:THR:O	1:C:499:ARG:NH1	2.40	0.54
1:B:72:LEU:HD12	1:B:116:LEU:HD22	1.90	0.53
1:G:475:THR:O	1:G:499:ARG:NH1	2.40	0.53
1:D:72:LEU:HD12	1:D:116:LEU:HD22	1.90	0.53
1:A:214:TRP:HB3	1:A:222:LEU:HD21	1.90	0.53
1:E:605:ASP:OD2	1:G:173:LYS:NZ	2.42	0.53
1:F:214:TRP:HB3	1:F:222:LEU:HD21	1.90	0.53
1:E:72:LEU:HD12	1:E:116:LEU:HD22	1.90	0.53
1:A:72:LEU:HD12	1:A:116:LEU:HD22	1.90	0.53
1:A:582:VAL:HG21	1:B:256:PRO:HD3	1.91	0.53
1:H:72:LEU:HD12	1:H:116:LEU:HD22	1.90	0.53
1:E:214:TRP:HB3	1:E:222:LEU:HD21	1.90	0.52
1:G:72:LEU:HD12	1:G:116:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LEU:HD12	1:C:116:LEU:HD22	1.90	0.52
1:D:214:TRP:HB3	1:D:222:LEU:HD21	1.90	0.52
1:F:72:LEU:HD12	1:F:116:LEU:HD22	1.90	0.52
1:G:214:TRP:HB3	1:G:222:LEU:HD21	1.90	0.52
1:H:214:TRP:HB3	1:H:222:LEU:HD21	1.90	0.52
1:D:564:VAL:HB	1:D:591:VAL:HG22	1.93	0.51
1:E:582:VAL:HG21	1:F:256:PRO:HD3	1.91	0.51
1:C:564:VAL:HB	1:C:591:VAL:HG22	1.93	0.51
1:E:564:VAL:HB	1:E:591:VAL:HG22	1.93	0.51
1:G:582:VAL:HG21	1:H:256:PRO:HD3	1.92	0.50
1:A:566:ILE:HG12	1:A:618:VAL:HB	1.93	0.50
1:H:566:ILE:HG12	1:H:618:VAL:HB	1.93	0.50
1:B:566:ILE:HG12	1:B:618:VAL:HB	1.93	0.50
1:A:334:LEU:HD22	1:A:377:LEU:HD11	1.94	0.50
1:B:564:VAL:HB	1:B:591:VAL:HG22	1.92	0.50
1:C:566:ILE:HG12	1:C:618:VAL:HB	1.93	0.50
1:B:334:LEU:HD22	1:B:377:LEU:HD11	1.94	0.50
1:G:334:LEU:HD22	1:G:377:LEU:HD11	1.94	0.50
1:H:564:VAL:HB	1:H:591:VAL:HG22	1.93	0.50
1:H:334:LEU:HD22	1:H:377:LEU:HD11	1.94	0.50
1:E:334:LEU:HD22	1:E:377:LEU:HD11	1.94	0.49
1:F:334:LEU:HD22	1:F:377:LEU:HD11	1.94	0.49
1:G:564:VAL:HB	1:G:591:VAL:HG22	1.93	0.49
1:F:564:VAL:HB	1:F:591:VAL:HG22	1.92	0.49
1:C:334:LEU:HD22	1:C:377:LEU:HD11	1.94	0.49
1:D:334:LEU:HD22	1:D:377:LEU:HD11	1.94	0.49
1:A:564:VAL:HB	1:A:591:VAL:HG22	1.93	0.49
1:E:129:LEU:HD21	1:E:147:LEU:HD23	1.95	0.49
1:G:566:ILE:HG12	1:G:618:VAL:HB	1.93	0.49
1:D:129:LEU:HD21	1:D:147:LEU:HD23	1.95	0.49
1:D:566:ILE:HG12	1:D:618:VAL:HB	1.93	0.49
1:F:129:LEU:HD21	1:F:147:LEU:HD23	1.95	0.49
1:G:129:LEU:HD21	1:G:147:LEU:HD23	1.94	0.49
1:C:129:LEU:HD21	1:C:147:LEU:HD23	1.95	0.49
1:E:566:ILE:HG12	1:E:618:VAL:HB	1.93	0.49
1:F:566:ILE:HG12	1:F:618:VAL:HB	1.93	0.49
1:B:129:LEU:HD21	1:B:147:LEU:HD23	1.95	0.48
1:G:523:LEU:HB3	1:G:529:ILE:HD12	1.96	0.48
1:G:235:LEU:HD22	1:G:329:ARG:HB3	1.96	0.48
1:H:235:LEU:HD22	1:H:329:ARG:HB3	1.96	0.48
1:C:322:ARG:NE	1:C:352:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ARG:NE	1:D:352:GLU:OE2	2.47	0.48
1:E:235:LEU:HD22	1:E:329:ARG:HB3	1.96	0.48
1:F:322:ARG:NE	1:F:352:GLU:OE2	2.47	0.48
1:G:158:ASP:OD1	1:G:194:HIS:NE2	2.47	0.48
1:H:129:LEU:HD21	1:H:147:LEU:HD23	1.95	0.48
1:A:129:LEU:HD21	1:A:147:LEU:HD23	1.95	0.48
1:E:322:ARG:NE	1:E:352:GLU:OE2	2.47	0.48
1:E:523:LEU:HB3	1:E:529:ILE:HD12	1.96	0.48
1:A:526:ASP:OD2	1:B:532:GLY:N	2.45	0.48
1:B:227:ALA:HB2	1:B:257:LEU:HD23	1.96	0.48
1:B:322:ARG:NE	1:B:352:GLU:OE2	2.47	0.48
1:F:523:LEU:HB3	1:F:529:ILE:HD12	1.96	0.48
1:A:227:ALA:HB2	1:A:257:LEU:HD23	1.96	0.47
1:D:227:ALA:HB2	1:D:257:LEU:HD23	1.96	0.47
1:D:523:LEU:HB3	1:D:529:ILE:HD12	1.96	0.47
1:A:158:ASP:OD1	1:A:194:HIS:NE2	2.47	0.47
1:E:339:LEU:HD11	1:E:383:ASN:HD22	1.80	0.47
1:G:322:ARG:NE	1:G:352:GLU:OE2	2.47	0.47
1:D:339:LEU:HD11	1:D:383:ASN:HD22	1.80	0.47
1:F:235:LEU:HD22	1:F:329:ARG:HB3	1.95	0.47
1:A:322:ARG:NE	1:A:352:GLU:OE2	2.47	0.47
1:F:339:LEU:HD11	1:F:383:ASN:HD22	1.80	0.47
1:G:339:LEU:HD11	1:G:383:ASN:HD22	1.80	0.47
1:A:523:LEU:HB3	1:A:529:ILE:HD12	1.96	0.47
1:B:246:VAL:HG11	1:B:283:VAL:HG13	1.97	0.47
1:H:322:ARG:NE	1:H:352:GLU:OE2	2.47	0.47
1:A:235:LEU:HD22	1:A:329:ARG:HB3	1.95	0.47
1:B:235:LEU:HD22	1:B:329:ARG:HB3	1.96	0.47
1:C:203:VAL:HG13	1:C:208:LEU:HD22	1.97	0.47
1:C:246:VAL:HG11	1:C:283:VAL:HG13	1.97	0.47
1:D:203:VAL:HG13	1:D:208:LEU:HD22	1.97	0.47
1:F:203:VAL:HG13	1:F:208:LEU:HD22	1.97	0.47
1:G:203:VAL:HG13	1:G:208:LEU:HD22	1.97	0.47
1:G:576:LEU:HD23	1:G:620:VAL:HG13	1.97	0.47
1:H:339:LEU:HD11	1:H:383:ASN:HD22	1.80	0.47
1:H:523:LEU:HB3	1:H:529:ILE:HD12	1.96	0.47
1:C:339:LEU:HD11	1:C:383:ASN:HD22	1.80	0.47
1:D:158:ASP:OD1	1:D:194:HIS:NE2	2.47	0.47
1:E:203:VAL:HG13	1:E:208:LEU:HD22	1.97	0.47
1:F:576:LEU:HD23	1:F:620:VAL:HG13	1.97	0.47
1:G:227:ALA:HB2	1:G:257:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:HD22	1:C:329:ARG:HB3	1.96	0.47
1:E:158:ASP:OD1	1:E:194:HIS:NE2	2.47	0.47
1:A:339:LEU:HD11	1:A:383:ASN:HD22	1.80	0.47
1:B:203:VAL:HG13	1:B:208:LEU:HD22	1.97	0.47
1:B:406:LEU:HD12	1:B:407:PRO:HD2	1.97	0.47
1:B:339:LEU:HD11	1:B:383:ASN:HD22	1.80	0.46
1:C:523:LEU:HB3	1:C:529:ILE:HD12	1.96	0.46
1:F:406:LEU:HD12	1:F:407:PRO:HD2	1.97	0.46
1:H:227:ALA:HB2	1:H:257:LEU:HD23	1.96	0.46
1:H:576:LEU:HD23	1:H:620:VAL:HG13	1.97	0.46
1:C:227:ALA:HB2	1:C:257:LEU:HD23	1.96	0.46
1:E:406:LEU:HD12	1:E:407:PRO:HD2	1.98	0.46
1:B:486:ASN:O	1:B:512:ARG:NH2	2.49	0.46
1:B:523:LEU:HB3	1:B:529:ILE:HD12	1.96	0.46
1:C:406:LEU:HD12	1:C:407:PRO:HD2	1.98	0.46
1:E:246:VAL:HG11	1:E:283:VAL:HG13	1.97	0.46
1:F:227:ALA:HB2	1:F:257:LEU:HD23	1.96	0.46
1:H:203:VAL:HG13	1:H:208:LEU:HD22	1.97	0.46
1:D:246:VAL:HG11	1:D:283:VAL:HG13	1.97	0.46
1:B:576:LEU:HD23	1:B:620:VAL:HG13	1.97	0.46
1:C:158:ASP:OD1	1:C:194:HIS:NE2	2.47	0.46
1:D:235:LEU:HD22	1:D:329:ARG:HB3	1.96	0.46
1:E:486:ASN:O	1:E:512:ARG:NH2	2.49	0.46
1:A:246:VAL:HG11	1:A:283:VAL:HG13	1.97	0.46
1:C:486:ASN:O	1:C:512:ARG:NH2	2.49	0.46
1:C:576:LEU:HD23	1:C:620:VAL:HG13	1.97	0.46
1:D:576:LEU:HD23	1:D:620:VAL:HG13	1.97	0.46
1:F:158:ASP:OD1	1:F:194:HIS:NE2	2.47	0.46
1:F:246:VAL:HG11	1:F:283:VAL:HG13	1.97	0.46
1:E:576:LEU:HD23	1:E:620:VAL:HG13	1.97	0.46
1:F:135:ALA:O	1:F:141:ARG:NH2	2.49	0.46
1:A:406:LEU:HD12	1:A:407:PRO:HD2	1.97	0.46
1:A:203:VAL:HG13	1:A:208:LEU:HD22	1.97	0.46
1:E:227:ALA:HB2	1:E:257:LEU:HD23	1.96	0.46
1:G:246:VAL:HG11	1:G:283:VAL:HG13	1.97	0.46
1:H:246:VAL:HG11	1:H:283:VAL:HG13	1.97	0.46
1:A:576:LEU:HD23	1:A:620:VAL:HG13	1.97	0.45
1:G:406:LEU:HD12	1:G:407:PRO:HD2	1.97	0.45
1:H:486:ASN:O	1:H:512:ARG:NH2	2.49	0.45
1:D:486:ASN:O	1:D:512:ARG:NH2	2.49	0.45
1:F:582:VAL:HG21	1:G:256:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:ASP:OD1	1:H:194:HIS:NE2	2.47	0.45
1:A:486:ASN:O	1:A:512:ARG:NH2	2.49	0.45
1:E:135:ALA:O	1:E:141:ARG:NH2	2.49	0.45
1:F:486:ASN:O	1:F:512:ARG:NH2	2.49	0.45
1:G:374:LEU:HD23	1:G:377:LEU:HD12	1.99	0.45
1:G:486:ASN:O	1:G:512:ARG:NH2	2.49	0.45
1:B:135:ALA:O	1:B:141:ARG:NH2	2.49	0.45
1:A:135:ALA:O	1:A:141:ARG:NH2	2.49	0.45
1:D:406:LEU:HD12	1:D:407:PRO:HD2	1.98	0.45
1:H:374:LEU:HD23	1:H:377:LEU:HD12	1.99	0.45
1:H:406:LEU:HD12	1:H:407:PRO:HD2	1.97	0.45
1:C:135:ALA:O	1:C:141:ARG:NH2	2.49	0.45
1:D:135:ALA:O	1:D:141:ARG:NH2	2.49	0.45
1:F:374:LEU:HD23	1:F:377:LEU:HD12	1.99	0.45
1:C:581:LYS:HD3	1:D:255:PHE:CE2	2.53	0.44
1:A:256:PRO:HD3	1:H:582:VAL:HG21	2.00	0.44
1:A:374:LEU:HD23	1:A:377:LEU:HD12	1.99	0.44
1:B:445:ARG:HE	1:C:464:LYS:HD3	1.83	0.44
1:E:374:LEU:HD23	1:E:377:LEU:HD12	1.99	0.44
1:B:465:ARG:HA	1:B:468:ARG:HE	1.83	0.44
1:D:465:ARG:HA	1:D:468:ARG:HE	1.83	0.44
1:E:692:ILE:HD13	1:E:695:ILE:HD12	2.00	0.44
1:F:692:ILE:HD13	1:F:695:ILE:HD12	2.00	0.44
1:C:374:LEU:HD23	1:C:377:LEU:HD12	1.99	0.43
1:D:383:ASN:HB3	1:D:386:LYS:HG2	2.01	0.43
1:H:465:ARG:HA	1:H:468:ARG:HE	1.83	0.43
1:H:135:ALA:O	1:H:141:ARG:NH2	2.49	0.43
1:A:692:ILE:HD13	1:A:695:ILE:HD12	2.00	0.43
1:B:374:LEU:HD23	1:B:377:LEU:HD12	1.99	0.43
1:B:692:ILE:HD13	1:B:695:ILE:HD12	2.00	0.43
1:C:605:ASP:OD2	1:E:173:LYS:NZ	2.42	0.43
1:D:692:ILE:HD13	1:D:695:ILE:HD12	2.00	0.43
1:G:465:ARG:HA	1:G:468:ARG:HE	1.83	0.43
1:C:383:ASN:HB3	1:C:386:LYS:HG2	2.00	0.43
1:C:412:TRP:HB2	1:C:440:GLY:HA3	2.01	0.43
1:E:383:ASN:HB3	1:E:386:LYS:HG2	2.01	0.43
1:B:158:ASP:OD1	1:B:194:HIS:NE2	2.47	0.43
1:C:526:ASP:OD2	1:D:532:GLY:N	2.51	0.43
1:D:374:LEU:HD23	1:D:377:LEU:HD12	1.99	0.43
1:E:465:ARG:HA	1:E:468:ARG:HE	1.83	0.43
1:F:383:ASN:HB3	1:F:386:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:412:TRP:HB2	1:H:440:GLY:HA3	2.01	0.43
1:A:465:ARG:HA	1:A:468:ARG:HE	1.83	0.43
1:E:526:ASP:OD2	1:F:532:GLY:N	2.50	0.43
1:F:593:ILE:HG21	1:G:255:PHE:HZ	1.84	0.43
1:A:412:TRP:HB2	1:A:440:GLY:HA3	2.01	0.42
1:D:582:VAL:HG21	1:E:256:PRO:HD3	2.00	0.42
1:G:692:ILE:HD13	1:G:695:ILE:HD12	2.00	0.42
1:B:383:ASN:HB3	1:B:386:LYS:HG2	2.00	0.42
1:B:412:TRP:HB2	1:B:440:GLY:HA3	2.01	0.42
1:C:465:ARG:HA	1:C:468:ARG:HE	1.83	0.42
1:C:621:LEU:HD12	1:C:657:ILE:HG13	2.02	0.42
1:C:692:ILE:HD13	1:C:695:ILE:HD12	2.00	0.42
1:B:621:LEU:HD12	1:B:657:ILE:HG13	2.02	0.42
1:F:465:ARG:HA	1:F:468:ARG:HE	1.83	0.42
1:G:412:TRP:HB2	1:G:440:GLY:HA3	2.01	0.42
1:D:412:TRP:HB2	1:D:440:GLY:HA3	2.01	0.42
1:E:412:TRP:HB2	1:E:440:GLY:HA3	2.01	0.42
1:H:692:ILE:HD13	1:H:695:ILE:HD12	2.00	0.42
1:D:621:LEU:HD12	1:D:657:ILE:HG13	2.02	0.42
1:G:383:ASN:HB3	1:G:386:LYS:HG2	2.01	0.42
1:A:383:ASN:HB3	1:A:386:LYS:HG2	2.00	0.42
1:F:412:TRP:HB2	1:F:440:GLY:HA3	2.01	0.42
1:H:383:ASN:HB3	1:H:386:LYS:HG2	2.01	0.42
1:F:109:GLY:HA2	1:F:112:VAL:HB	2.02	0.42
1:B:109:GLY:HA2	1:B:112:VAL:HB	2.02	0.42
1:C:109:GLY:HA2	1:C:112:VAL:HB	2.02	0.42
1:E:109:GLY:HA2	1:E:112:VAL:HB	2.02	0.41
1:A:109:GLY:HA2	1:A:112:VAL:HB	2.02	0.41
1:A:621:LEU:HD12	1:A:657:ILE:HG13	2.02	0.41
1:G:109:GLY:HA2	1:G:112:VAL:HB	2.02	0.41
1:E:621:LEU:HD12	1:E:657:ILE:HG13	2.02	0.41
1:G:581:LYS:HG3	1:G:591:VAL:HB	2.02	0.41
1:G:581:LYS:HD3	1:H:255:PHE:CE2	2.56	0.41
1:F:581:LYS:HG3	1:F:591:VAL:HB	2.02	0.41
1:H:621:LEU:HD12	1:H:657:ILE:HG13	2.02	0.41
1:D:109:GLY:HA2	1:D:112:VAL:HB	2.02	0.41
1:E:276:VAL:HG22	1:E:333:LEU:HD21	2.03	0.41
1:E:445:ARG:HE	1:F:464:LYS:HD3	1.86	0.41
1:E:529:ILE:O	1:E:535:ARG:NH1	2.48	0.41
1:F:150:GLN:NE2	2:F:1000:NAD:H2N	2.36	0.41
1:H:109:GLY:HA2	1:H:112:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:HD13	1:B:338:ARG:HH11	1.86	0.41
1:C:293:LEU:HD13	1:C:338:ARG:HH11	1.86	0.41
1:D:293:LEU:HD13	1:D:338:ARG:HH11	1.86	0.41
1:D:529:ILE:O	1:D:535:ARG:NH1	2.48	0.41
1:E:581:LYS:HG3	1:E:591:VAL:HB	2.02	0.41
1:G:135:ALA:O	1:G:141:ARG:NH2	2.49	0.41
1:H:581:LYS:HG3	1:H:591:VAL:HB	2.02	0.41
1:A:293:LEU:HD13	1:A:338:ARG:HH11	1.86	0.41
1:B:276:VAL:HG22	1:B:333:LEU:HD21	2.03	0.41
1:C:276:VAL:HG22	1:C:333:LEU:HD21	2.03	0.41
1:C:581:LYS:HG3	1:C:591:VAL:HB	2.02	0.41
1:F:293:LEU:HD13	1:F:338:ARG:HH11	1.86	0.41
1:F:621:LEU:HD12	1:F:657:ILE:HG13	2.02	0.41
1:G:621:LEU:HD12	1:G:657:ILE:HG13	2.02	0.41
1:A:276:VAL:HG22	1:A:333:LEU:HD21	2.03	0.41
1:A:445:ARG:HE	1:B:464:LYS:HD3	1.86	0.41
1:B:581:LYS:HG3	1:B:591:VAL:HB	2.02	0.41
1:G:276:VAL:HG22	1:G:333:LEU:HD21	2.03	0.40
1:G:445:ARG:HE	1:H:464:LYS:HD3	1.86	0.40
1:A:581:LYS:HG3	1:A:591:VAL:HB	2.02	0.40
1:D:581:LYS:HG3	1:D:591:VAL:HB	2.02	0.40
1:D:276:VAL:HG22	1:D:333:LEU:HD21	2.03	0.40
1:G:293:LEU:HD13	1:G:338:ARG:HH11	1.86	0.40
1:A:150:GLN:NE2	2:A:1000:NAD:H2N	2.36	0.40
1:B:223:LEU:HB2	1:B:266:LEU:HD11	2.04	0.40
1:C:223:LEU:HB2	1:C:266:LEU:HD11	2.04	0.40
1:D:223:LEU:HB2	1:D:266:LEU:HD11	2.04	0.40
1:E:223:LEU:HB2	1:E:266:LEU:HD11	2.04	0.40
1:F:529:ILE:O	1:F:535:ARG:NH1	2.48	0.40
1:H:293:LEU:HD13	1:H:338:ARG:HH11	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
1	B	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
1	C	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
1	D	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
1	E	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
1	F	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
1	G	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
1	H	614/733 (84%)	589 (96%)	25 (4%)	0	100	100
All	All	4912/5864 (84%)	4712 (96%)	200 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/598 (86%)	516 (100%)	0	100	100
1	B	516/598 (86%)	516 (100%)	0	100	100
1	C	516/598 (86%)	516 (100%)	0	100	100
1	D	516/598 (86%)	516 (100%)	0	100	100
1	E	516/598 (86%)	516 (100%)	0	100	100
1	F	516/598 (86%)	516 (100%)	0	100	100
1	G	516/598 (86%)	516 (100%)	0	100	100
1	H	516/598 (86%)	516 (100%)	0	100	100
All	All	4128/4784 (86%)	4128 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	583	HIS
1	B	583	HIS
1	C	583	HIS
1	F	583	HIS
1	G	583	HIS
1	H	583	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	F	1000	-	42,48,48	0.76	1 (2%)	50,73,73	0.81	1 (2%)
2	NAD	H	1000	-	42,48,48	0.76	1 (2%)	50,73,73	0.82	1 (2%)
2	NAD	C	1000	-	42,48,48	0.76	1 (2%)	50,73,73	0.82	1 (2%)
2	NAD	A	1000	-	42,48,48	0.76	1 (2%)	50,73,73	0.82	1 (2%)
2	NAD	G	1000	-	42,48,48	0.76	1 (2%)	50,73,73	0.82	1 (2%)
2	NAD	D	1000	-	42,48,48	0.75	1 (2%)	50,73,73	0.82	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	E	1000	-	42,48,48	0.76	1 (2%)	50,73,73	0.83	1 (2%)
2	NAD	B	1000	-	42,48,48	0.76	1 (2%)	50,73,73	0.81	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	F	1000	-	-	9/26/62/62	0/5/5/5
2	NAD	H	1000	-	-	8/26/62/62	0/5/5/5
2	NAD	C	1000	-	-	9/26/62/62	0/5/5/5
2	NAD	A	1000	-	-	9/26/62/62	0/5/5/5
2	NAD	G	1000	-	-	9/26/62/62	0/5/5/5
2	NAD	D	1000	-	-	9/26/62/62	0/5/5/5
2	NAD	E	1000	-	-	9/26/62/62	0/5/5/5
2	NAD	B	1000	-	-	8/26/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	NAD	O2D-C2D	2.27	1.48	1.43
2	A	1000	NAD	O2D-C2D	2.26	1.48	1.43
2	F	1000	NAD	O2D-C2D	2.24	1.48	1.43
2	H	1000	NAD	O2D-C2D	2.23	1.48	1.43
2	G	1000	NAD	O2D-C2D	2.23	1.48	1.43
2	E	1000	NAD	O2D-C2D	2.23	1.48	1.43
2	D	1000	NAD	O2D-C2D	2.22	1.48	1.43
2	B	1000	NAD	O2D-C2D	2.21	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1000	NAD	N3A-C2A-N1A	-2.26	125.14	128.68
2	C	1000	NAD	N3A-C2A-N1A	-2.24	125.18	128.68
2	B	1000	NAD	N3A-C2A-N1A	-2.23	125.19	128.68
2	E	1000	NAD	N3A-C2A-N1A	-2.23	125.19	128.68
2	A	1000	NAD	N3A-C2A-N1A	-2.22	125.21	128.68
2	D	1000	NAD	N3A-C2A-N1A	-2.21	125.23	128.68
2	H	1000	NAD	N3A-C2A-N1A	-2.21	125.23	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1000	NAD	N3A-C2A-N1A	-2.19	125.25	128.68

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	NAD	C5B-O5B-PA-O1A
2	B	1000	NAD	C5B-O5B-PA-O1A
2	C	1000	NAD	C5B-O5B-PA-O1A
2	D	1000	NAD	C5B-O5B-PA-O1A
2	E	1000	NAD	C5B-O5B-PA-O1A
2	G	1000	NAD	C5B-O5B-PA-O1A
2	H	1000	NAD	C5B-O5B-PA-O1A
2	A	1000	NAD	O4B-C4B-C5B-O5B
2	A	1000	NAD	C3B-C4B-C5B-O5B
2	B	1000	NAD	O4B-C4B-C5B-O5B
2	B	1000	NAD	C3B-C4B-C5B-O5B
2	C	1000	NAD	O4B-C4B-C5B-O5B
2	C	1000	NAD	C3B-C4B-C5B-O5B
2	D	1000	NAD	O4B-C4B-C5B-O5B
2	D	1000	NAD	C3B-C4B-C5B-O5B
2	E	1000	NAD	O4B-C4B-C5B-O5B
2	E	1000	NAD	C3B-C4B-C5B-O5B
2	F	1000	NAD	O4B-C4B-C5B-O5B
2	F	1000	NAD	C3B-C4B-C5B-O5B
2	G	1000	NAD	O4B-C4B-C5B-O5B
2	G	1000	NAD	C3B-C4B-C5B-O5B
2	H	1000	NAD	O4B-C4B-C5B-O5B
2	H	1000	NAD	C3B-C4B-C5B-O5B
2	E	1000	NAD	C3D-C4D-C5D-O5D
2	F	1000	NAD	C3D-C4D-C5D-O5D
2	C	1000	NAD	C3D-C4D-C5D-O5D
2	D	1000	NAD	C3D-C4D-C5D-O5D
2	A	1000	NAD	C4B-C5B-O5B-PA
2	B	1000	NAD	C4B-C5B-O5B-PA
2	C	1000	NAD	C4B-C5B-O5B-PA
2	D	1000	NAD	C4B-C5B-O5B-PA
2	E	1000	NAD	C4B-C5B-O5B-PA
2	F	1000	NAD	C4B-C5B-O5B-PA
2	G	1000	NAD	C4B-C5B-O5B-PA
2	H	1000	NAD	C4B-C5B-O5B-PA
2	A	1000	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	B	1000	NAD	C5B-O5B-PA-O3
2	C	1000	NAD	C5B-O5B-PA-O3
2	D	1000	NAD	C5B-O5B-PA-O3
2	E	1000	NAD	C5B-O5B-PA-O3
2	F	1000	NAD	C5B-O5B-PA-O3
2	G	1000	NAD	C5B-O5B-PA-O3
2	H	1000	NAD	C5B-O5B-PA-O3
2	G	1000	NAD	C3D-C4D-C5D-O5D
2	A	1000	NAD	C5B-O5B-PA-O2A
2	B	1000	NAD	C5B-O5B-PA-O2A
2	C	1000	NAD	C5B-O5B-PA-O2A
2	D	1000	NAD	C5B-O5B-PA-O2A
2	E	1000	NAD	C5B-O5B-PA-O2A
2	F	1000	NAD	C5B-O5B-PA-O1A
2	F	1000	NAD	C5B-O5B-PA-O2A
2	G	1000	NAD	C5B-O5B-PA-O2A
2	H	1000	NAD	C5B-O5B-PA-O2A
2	A	1000	NAD	C3D-C4D-C5D-O5D
2	H	1000	NAD	C3D-C4D-C5D-O5D
2	B	1000	NAD	C3D-C4D-C5D-O5D
2	E	1000	NAD	O4D-C4D-C5D-O5D
2	F	1000	NAD	O4D-C4D-C5D-O5D
2	D	1000	NAD	O4D-C4D-C5D-O5D
2	C	1000	NAD	O4D-C4D-C5D-O5D
2	A	1000	NAD	C5D-O5D-PN-O1N
2	B	1000	NAD	C5D-O5D-PN-O1N
2	C	1000	NAD	C5D-O5D-PN-O1N
2	D	1000	NAD	C5D-O5D-PN-O1N
2	E	1000	NAD	C5D-O5D-PN-O1N
2	F	1000	NAD	C5D-O5D-PN-O1N
2	G	1000	NAD	C5D-O5D-PN-O1N
2	H	1000	NAD	C5D-O5D-PN-O1N
2	A	1000	NAD	O4D-C4D-C5D-O5D
2	G	1000	NAD	O4D-C4D-C5D-O5D

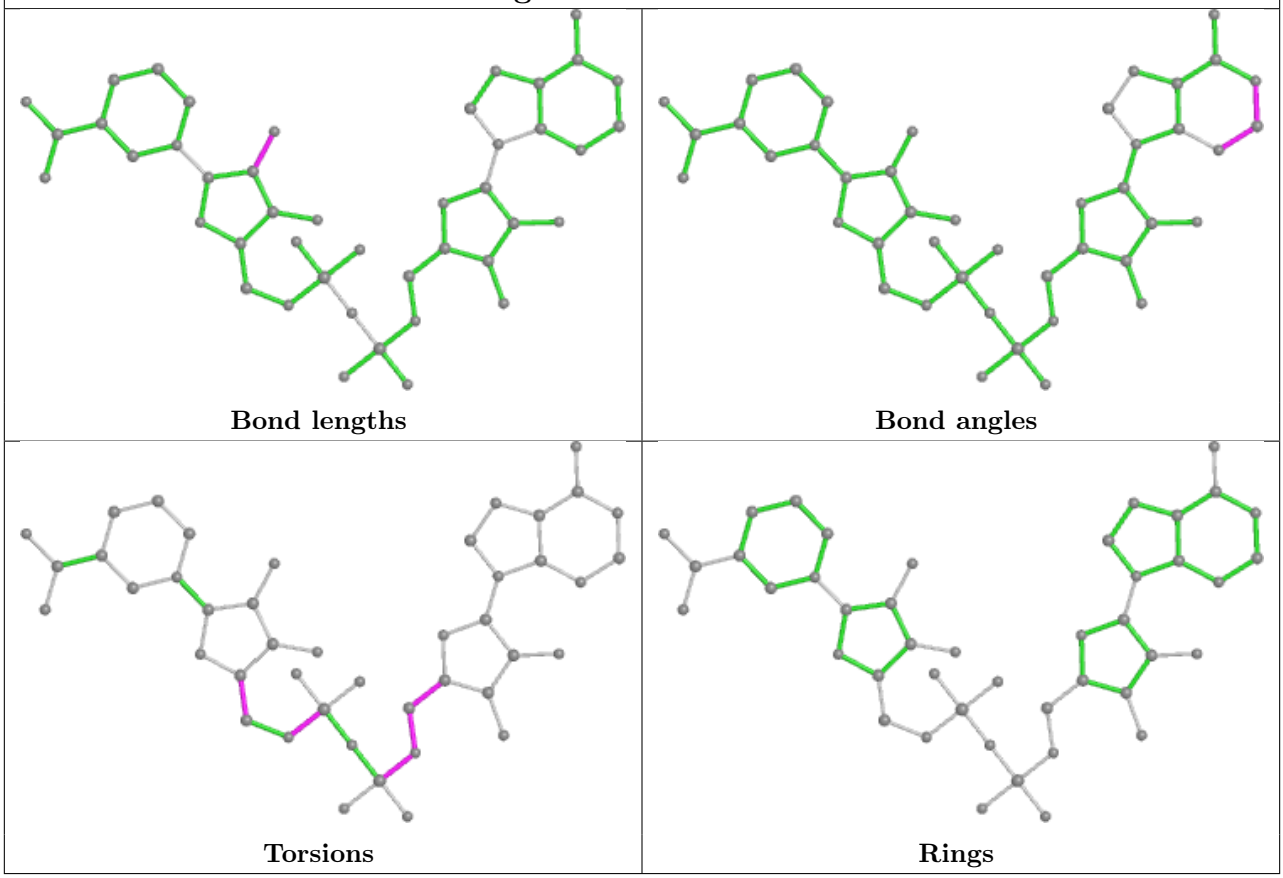
There are no ring outliers.

2 monomers are involved in 2 short contacts:

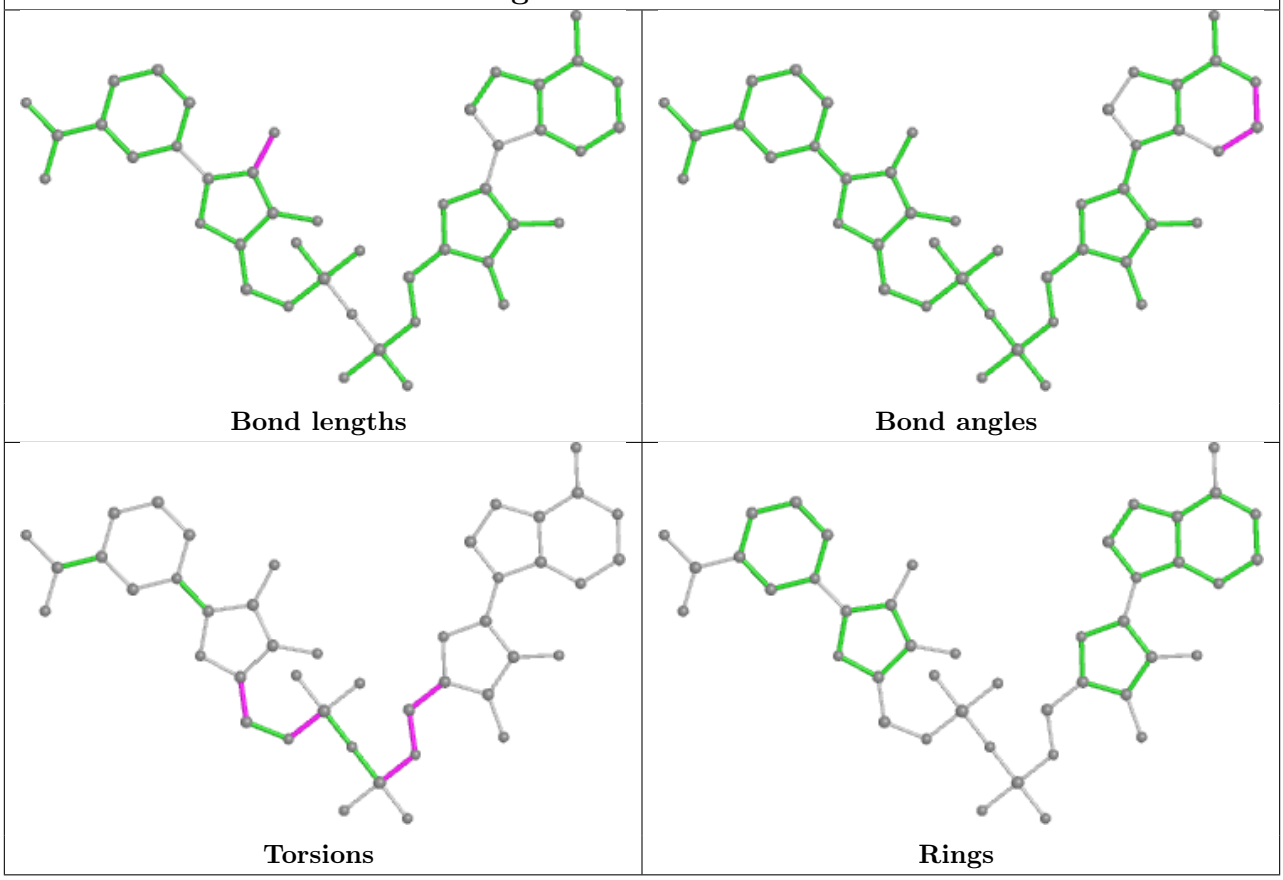
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1000	NAD	1	0
2	A	1000	NAD	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

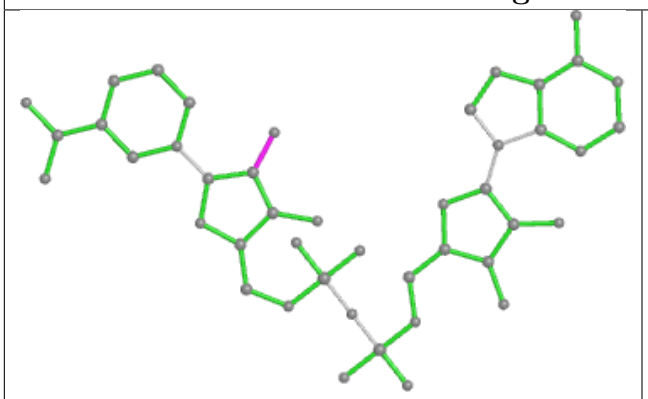
Ligand NAD F 1000



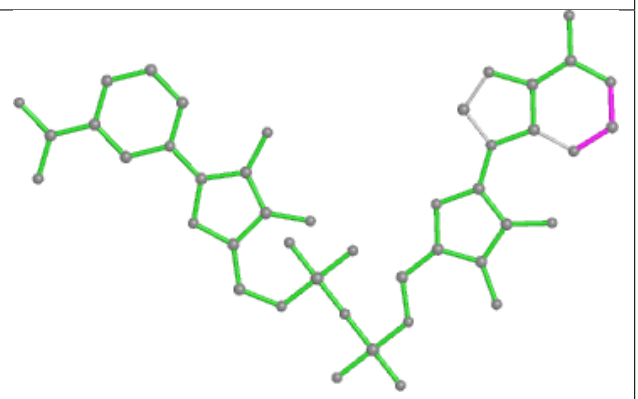
Ligand NAD H 1000



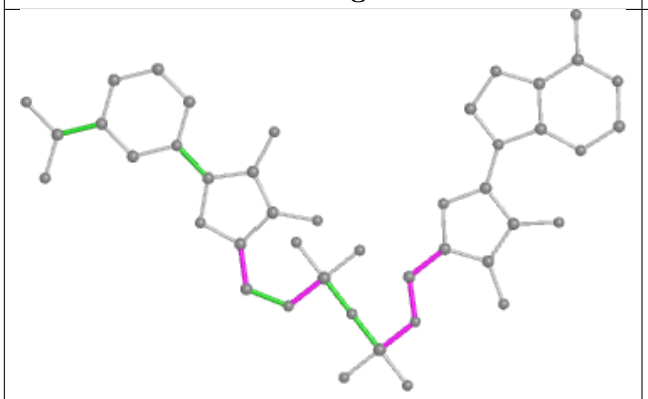
Ligand NAD C 1000



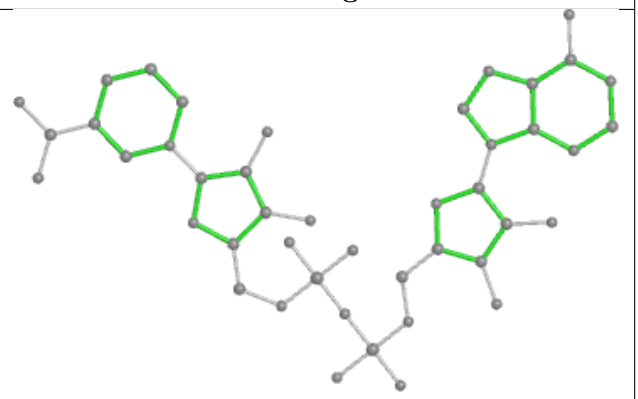
Bond lengths



Bond angles

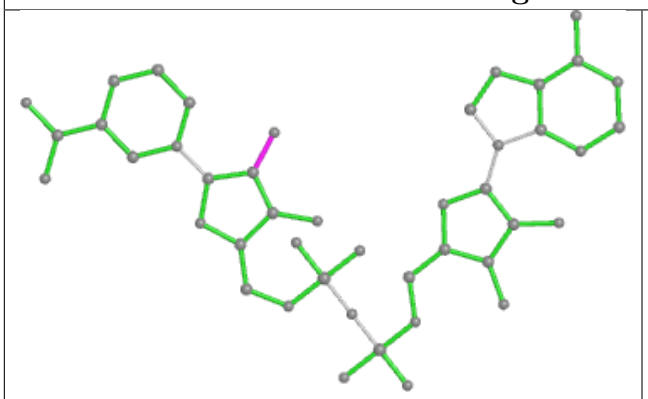


Torsions

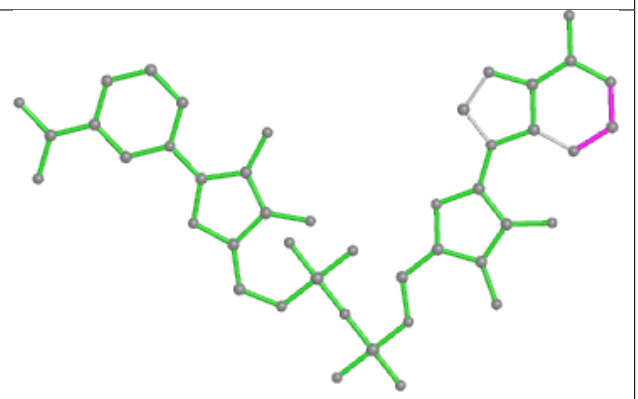


Rings

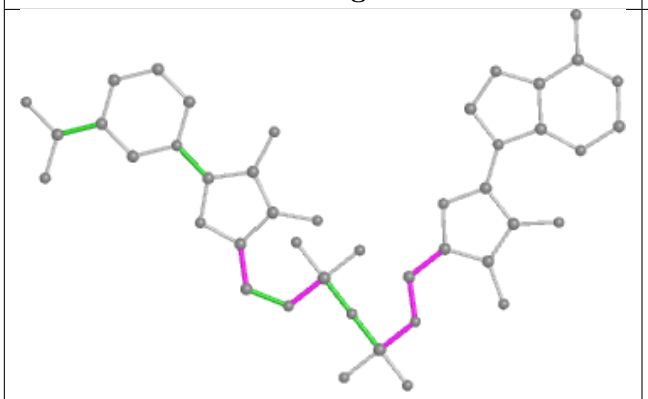
Ligand NAD A 1000



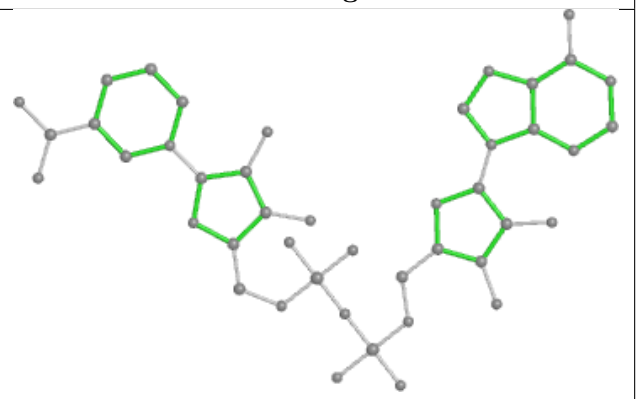
Bond lengths



Bond angles

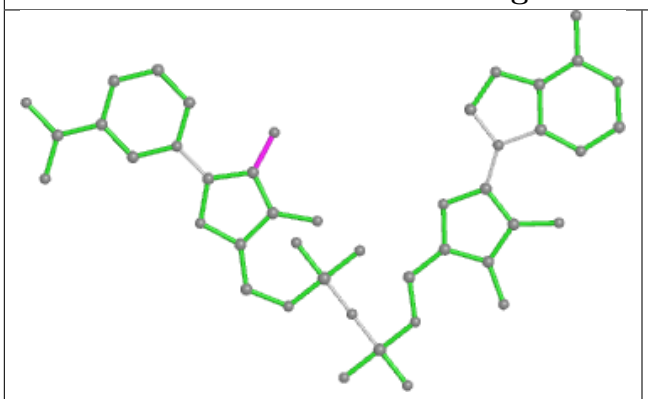


Torsions

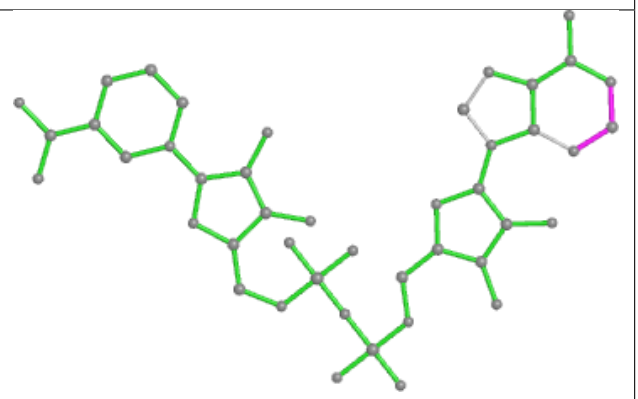


Rings

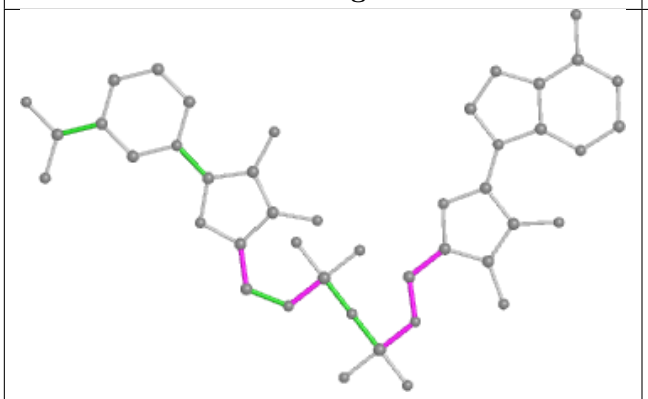
Ligand NAD G 1000



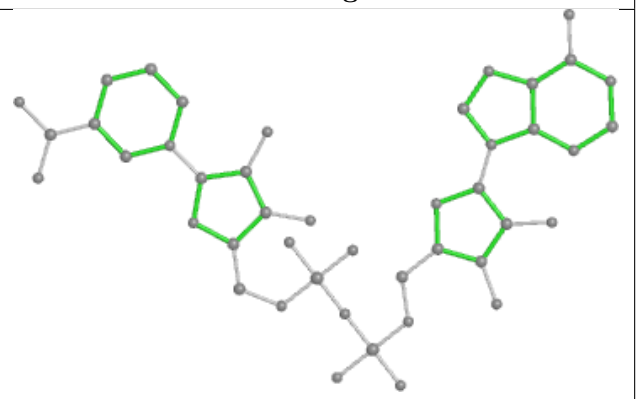
Bond lengths



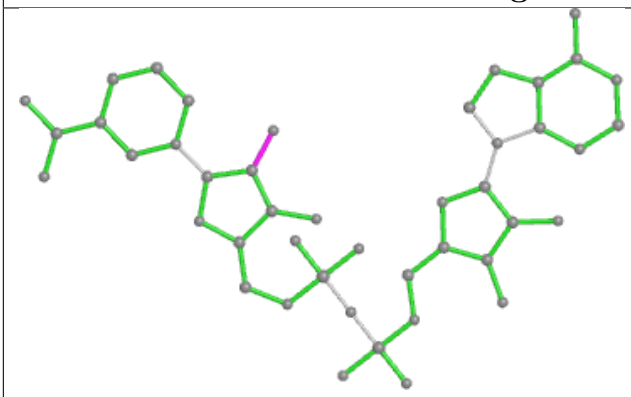
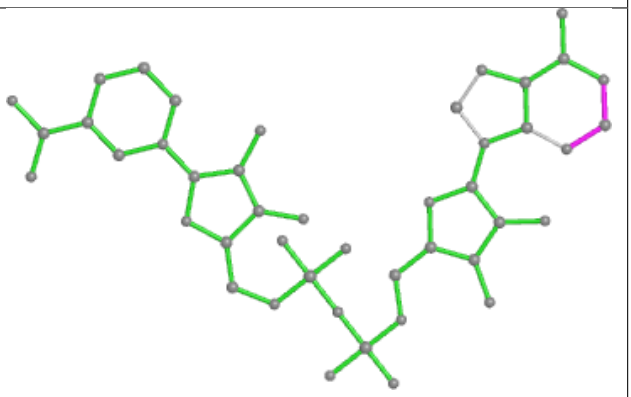
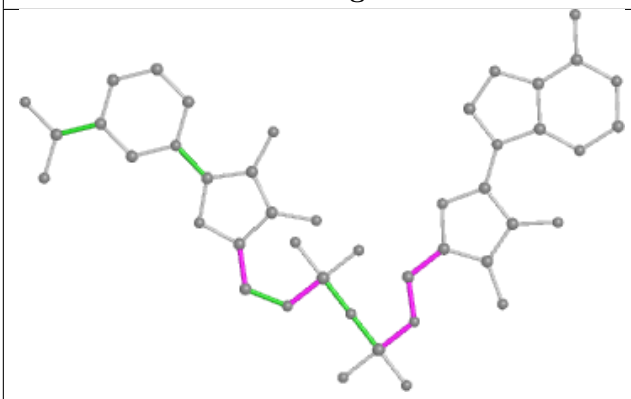
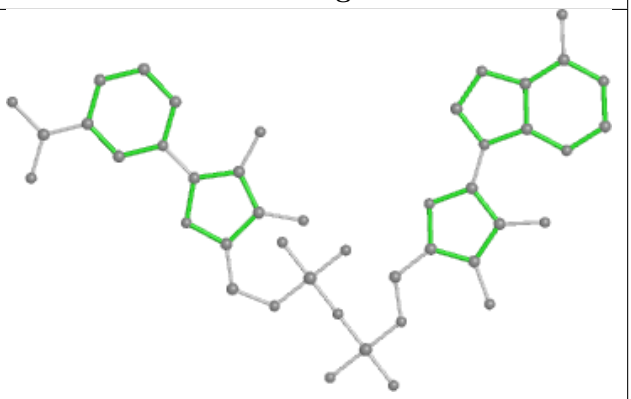
Bond angles

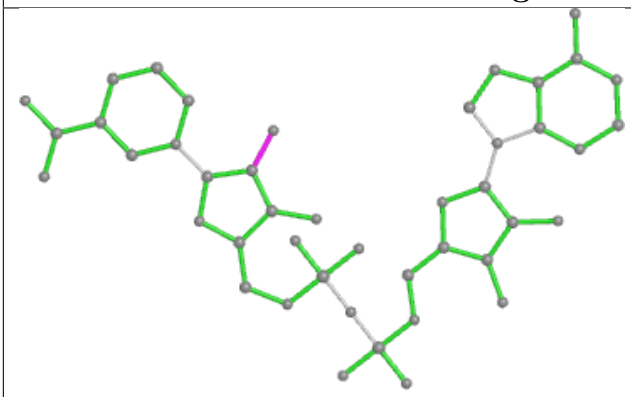
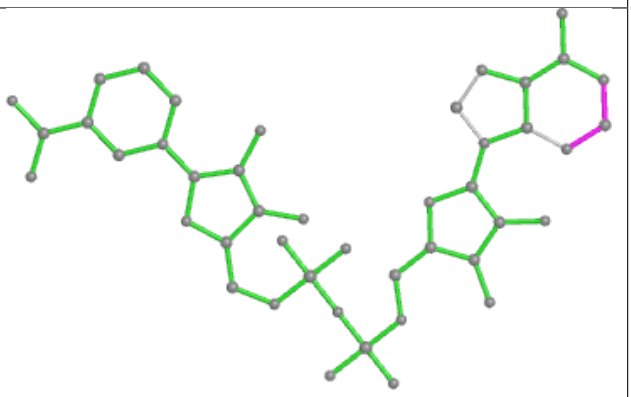
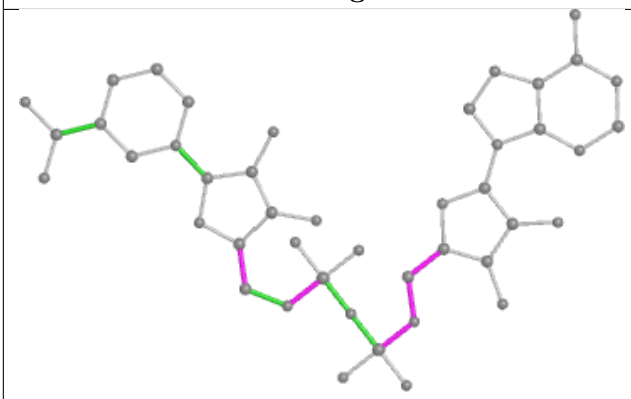
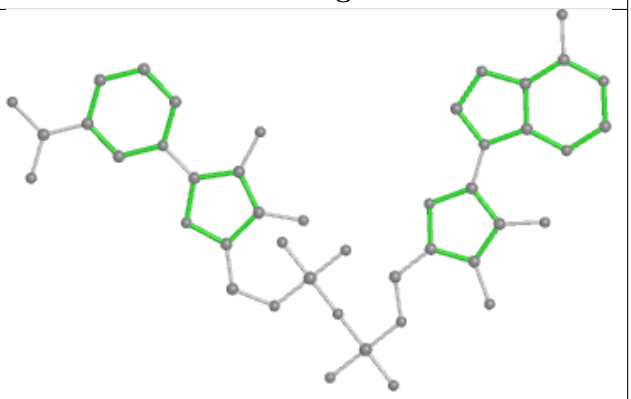


Torsions

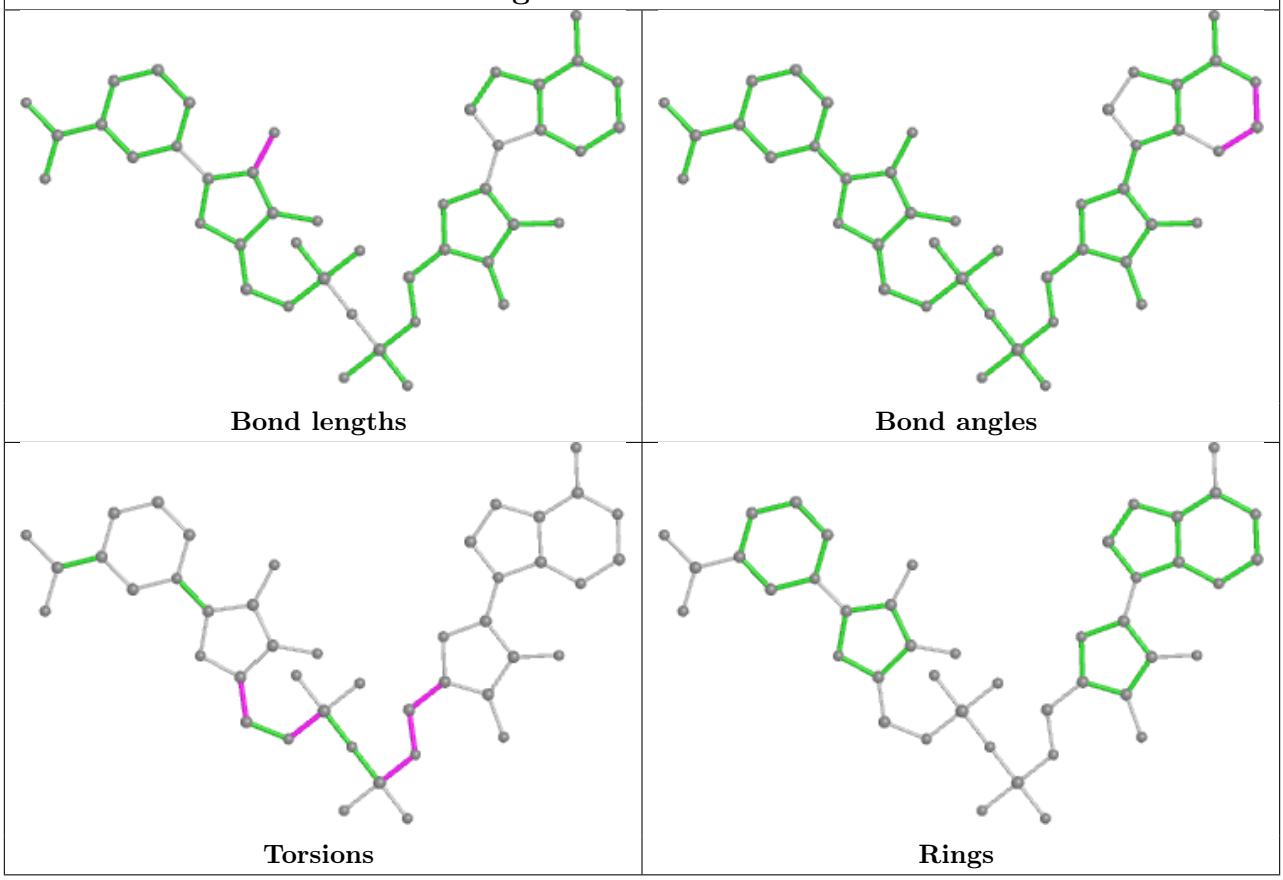


Rings

Ligand NAD D 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAD E 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAD B 1000



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.

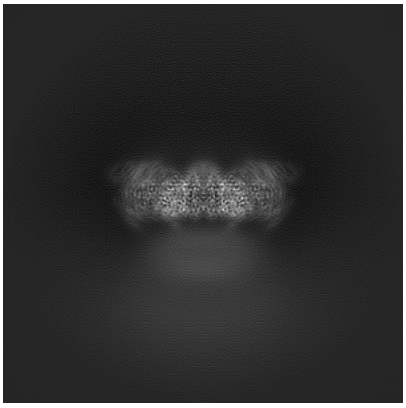
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30403. 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



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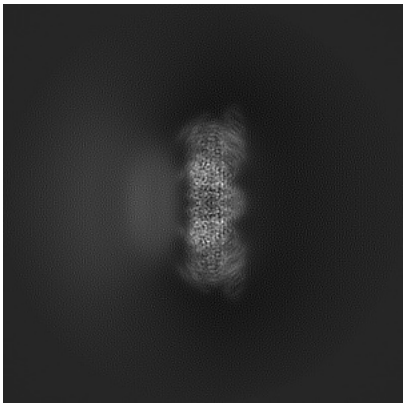
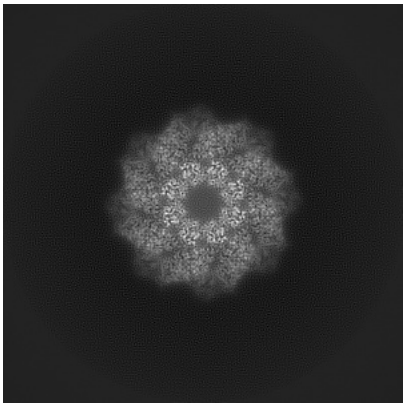


Y

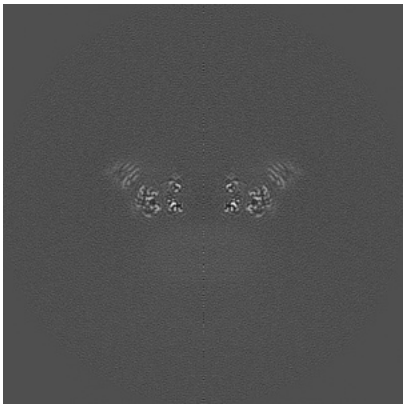


Z

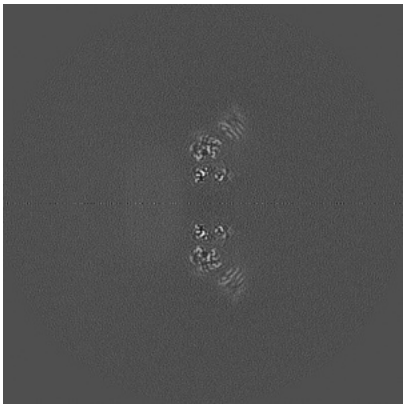
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

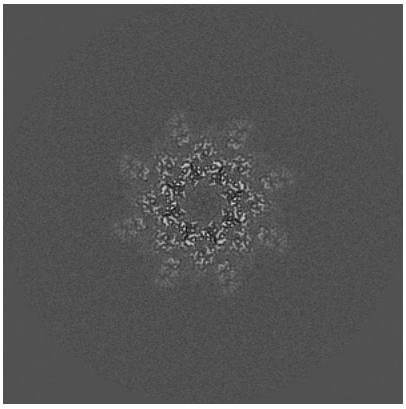
6.2.1 Primary map



X Index: 192



Y Index: 192

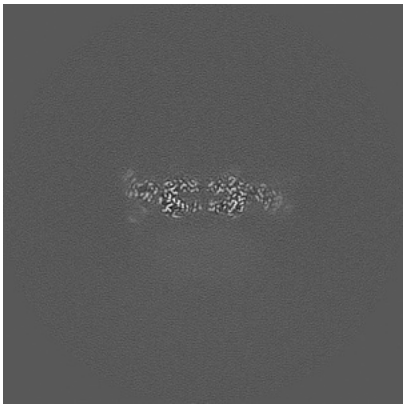


Z Index: 192

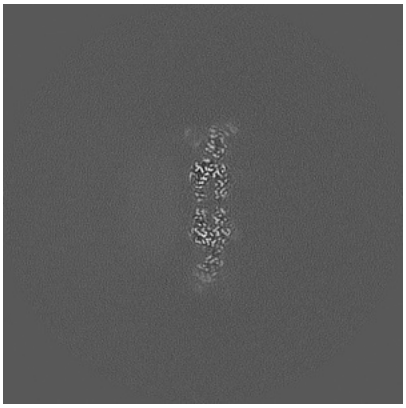
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

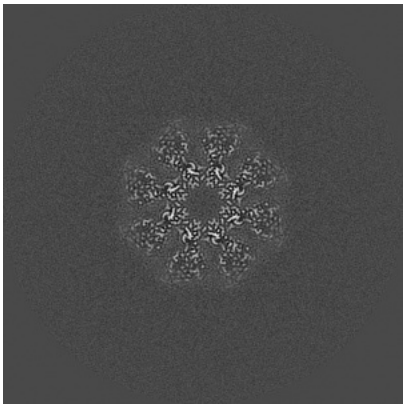
6.3.1 Primary map



X Index: 174



Y Index: 174

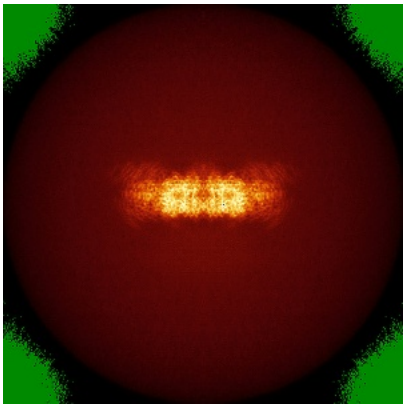


Z Index: 205

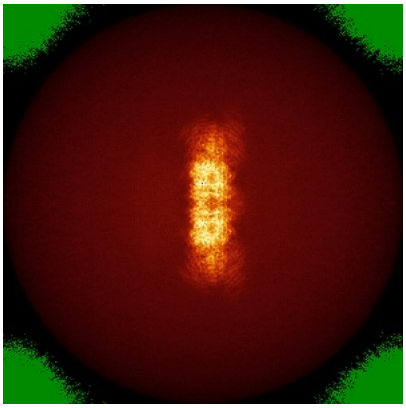
The images above show the largest variance slices of the map in three orthogonal directions.

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

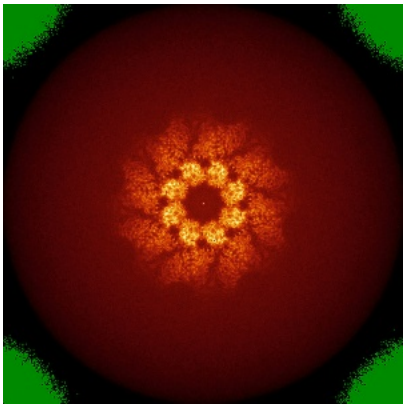
6.4.1 Primary map



X



Y

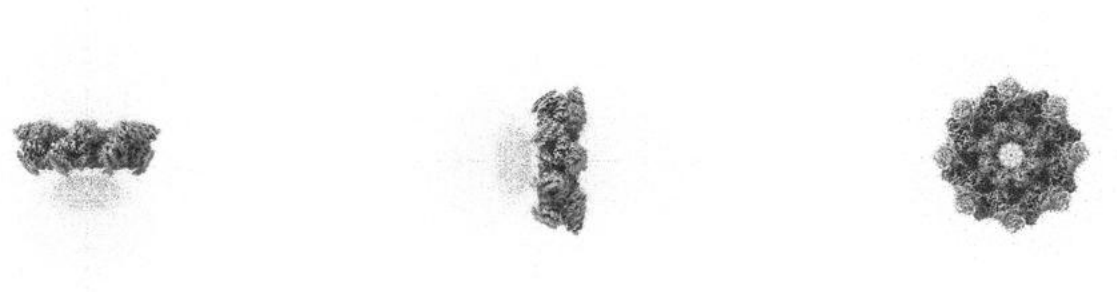


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

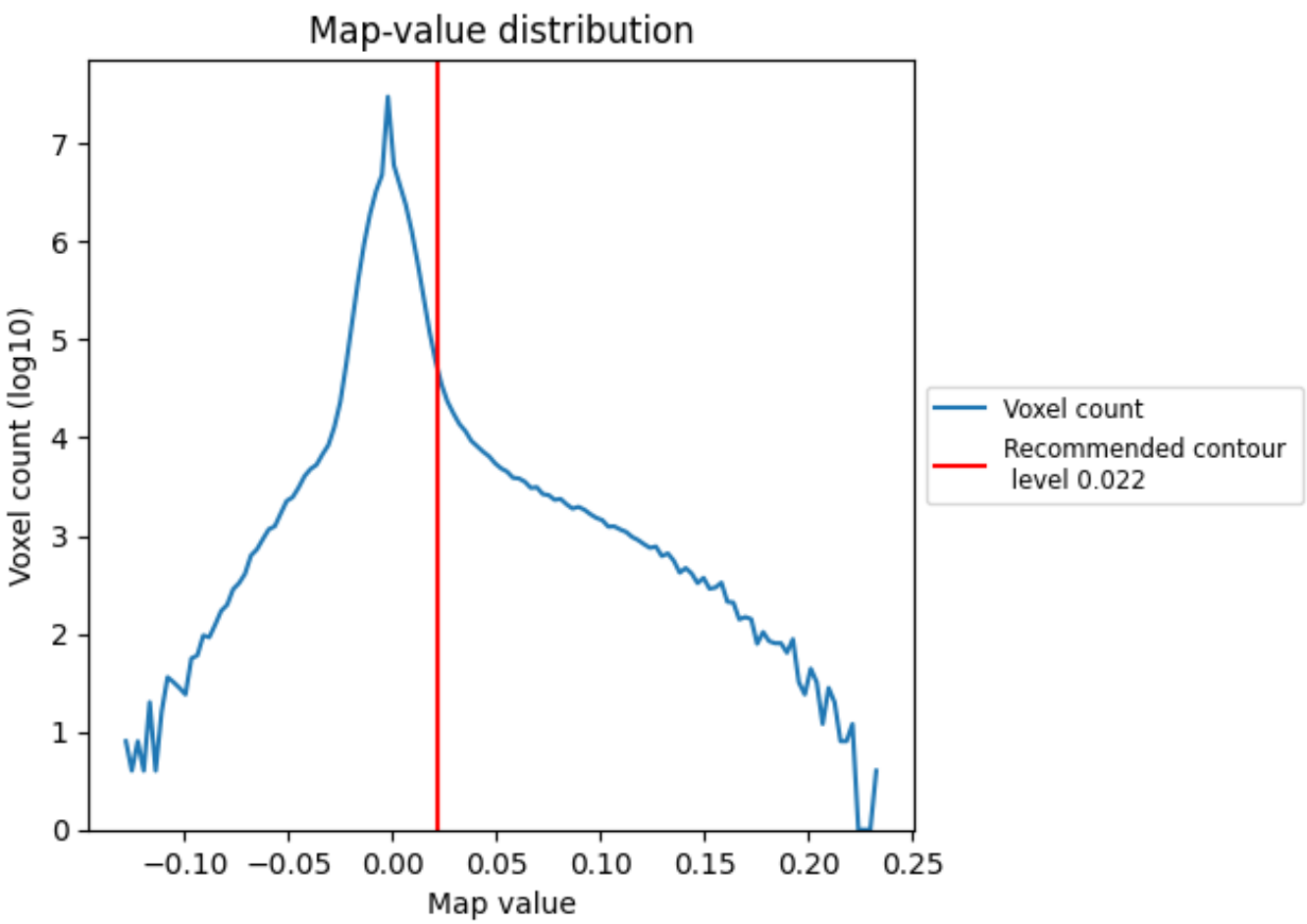
6.6 Mask visualisation (i)

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

7 Map analysis (i)

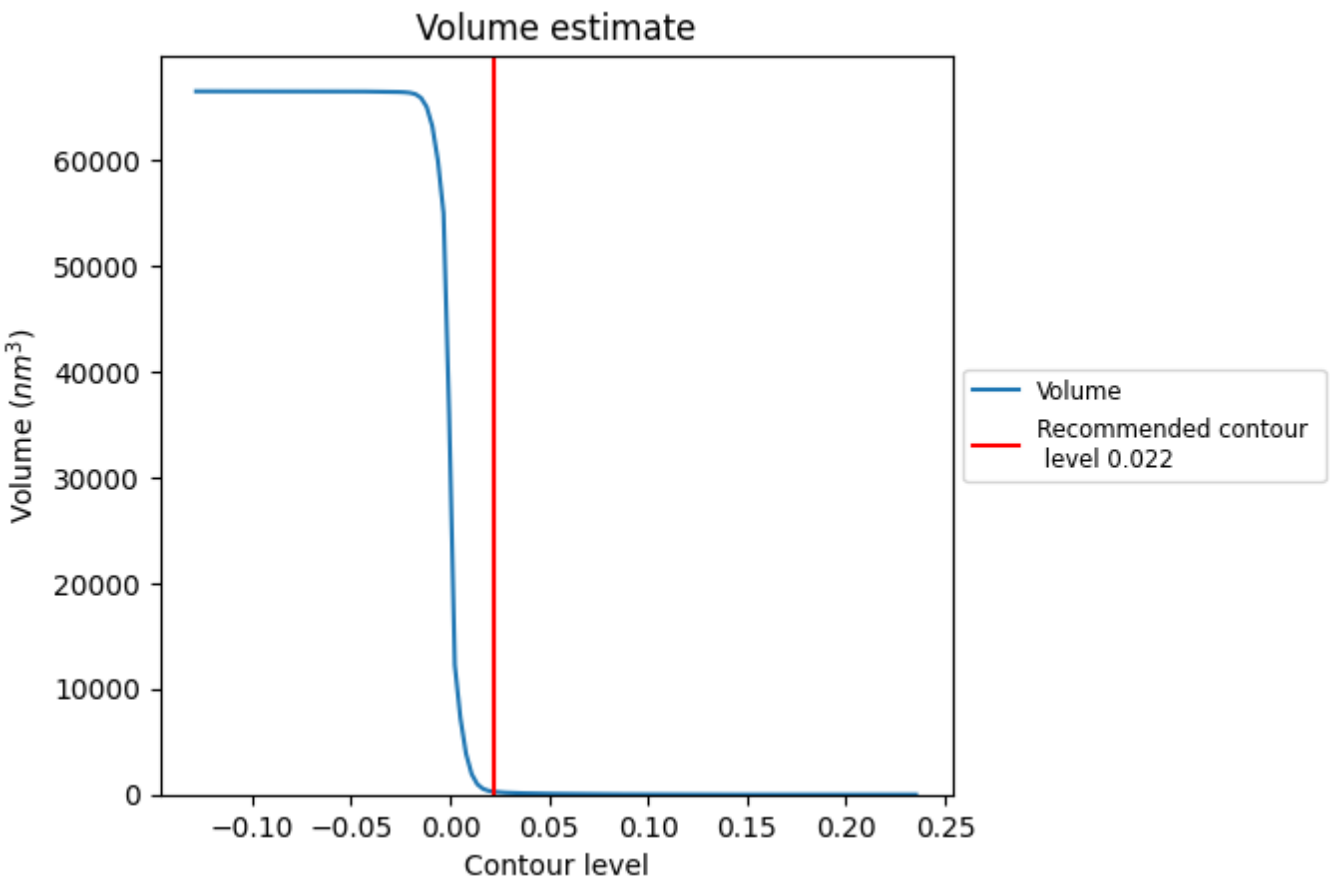
This section contains the results of statistical analysis of the map.

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.

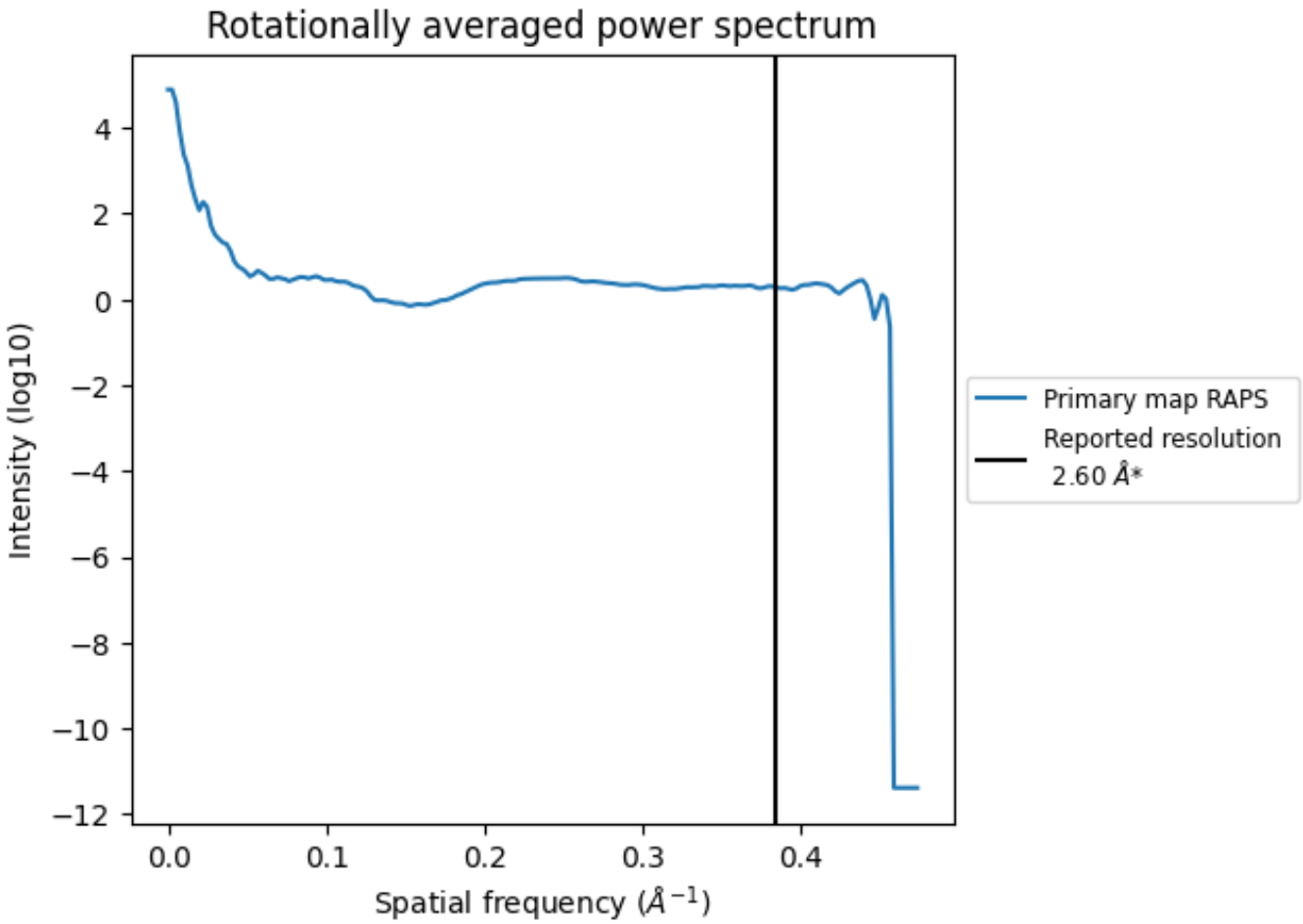
7.2 Volume estimate (i)



The volume at the recommended contour level is 275 nm^3; this corresponds to an approximate mass of 248 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 0.385 Å^{-1}

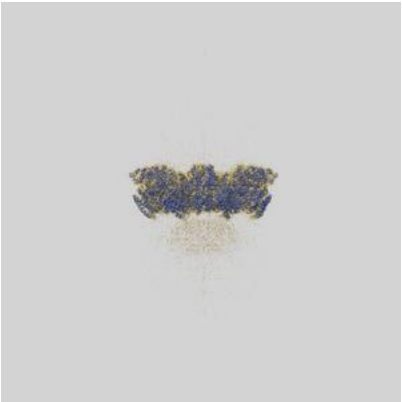
8 Fourier-Shell correlation (i)

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

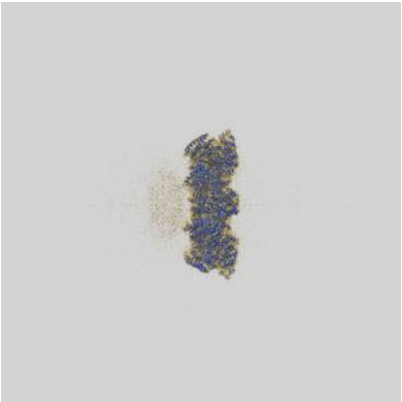
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30403 and PDB model 7CM7. Per-residue inclusion information can be found in section 3 on page 7.

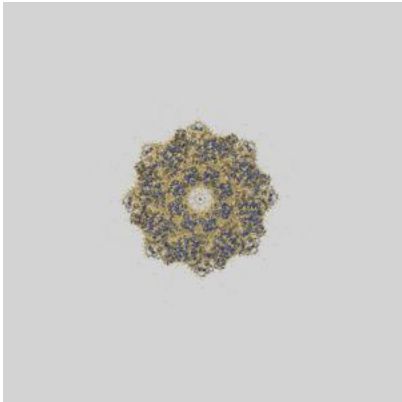
9.1 Map-model overlay (i)



X



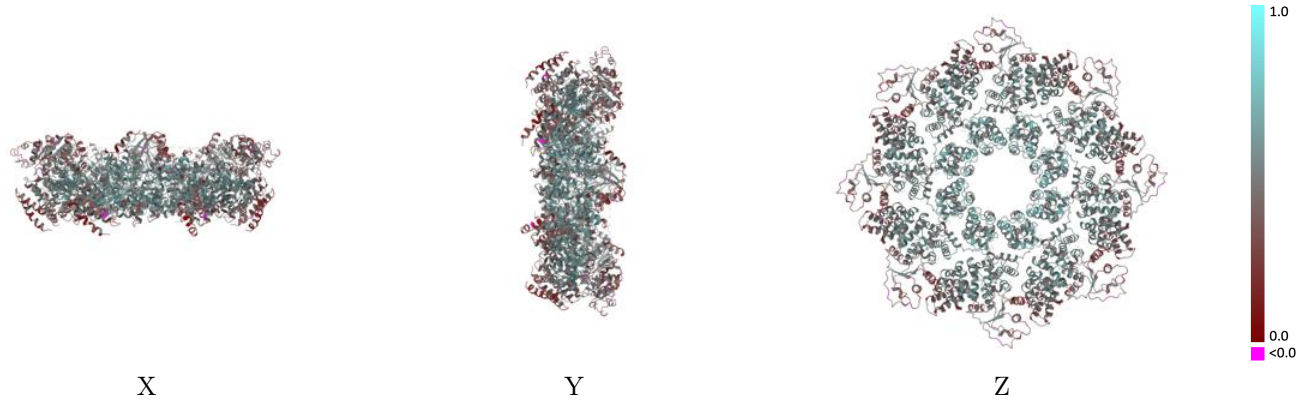
Y



Z

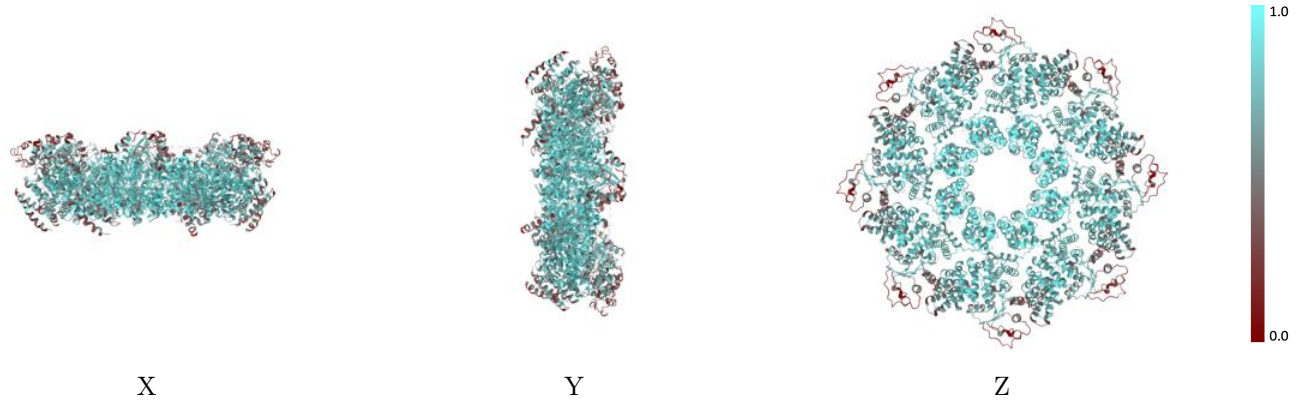
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



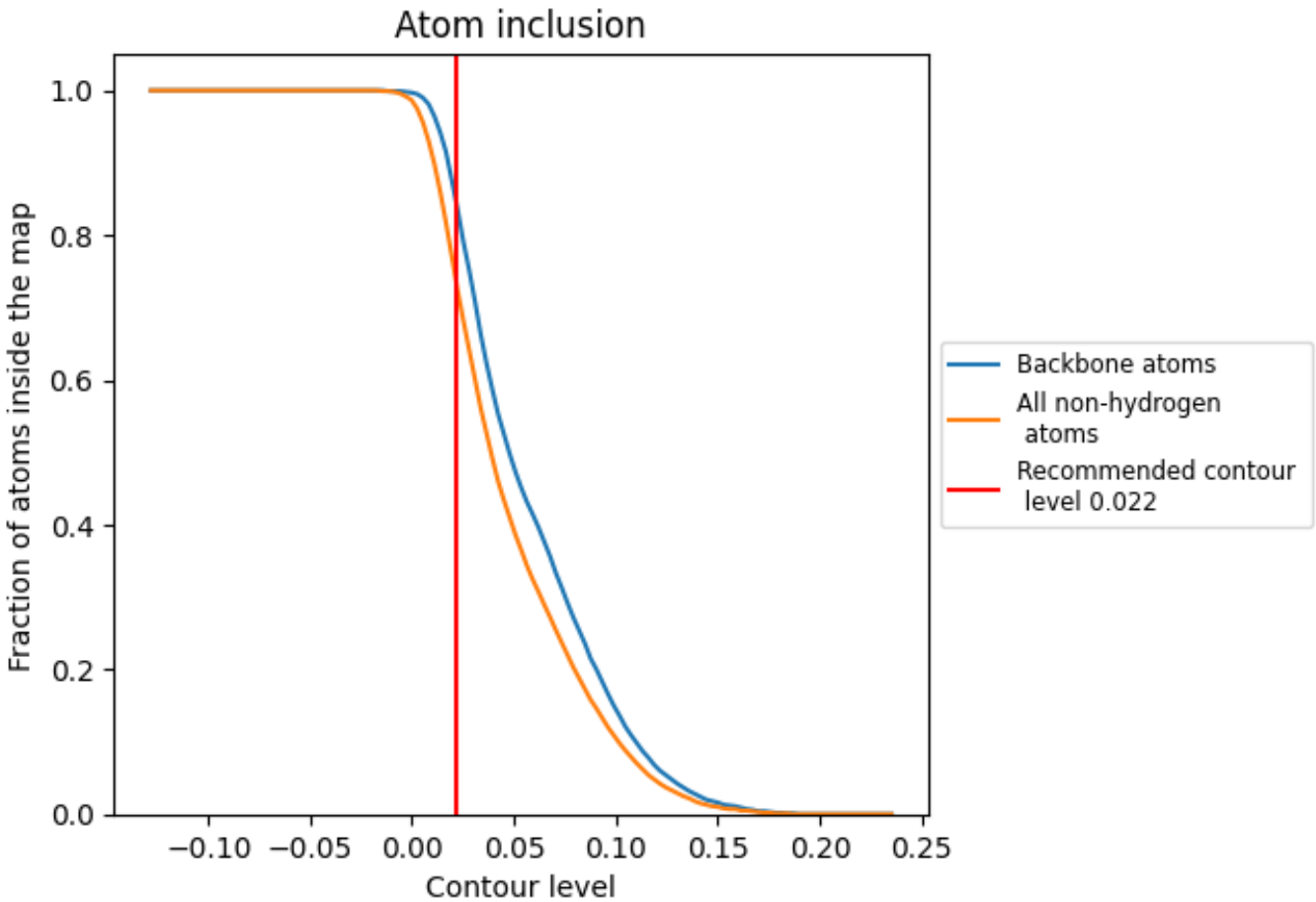
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7290	0.4760
A	0.7300	0.4750
B	0.7290	0.4740
C	0.7290	0.4750
D	0.7270	0.4760
E	0.7290	0.4770
F	0.7300	0.4760
G	0.7300	0.4770
H	0.7300	0.4760