Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 07:08 pm BST

PDB ID	:	8ATI
Title	:	Human CtBP2(31-364) in complex with RAI2 peptide(315-322)
Authors	:	Mullapudi, E.; Goradia, N.; Wilmanns, M.
Deposited on	:	2022-08-23
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

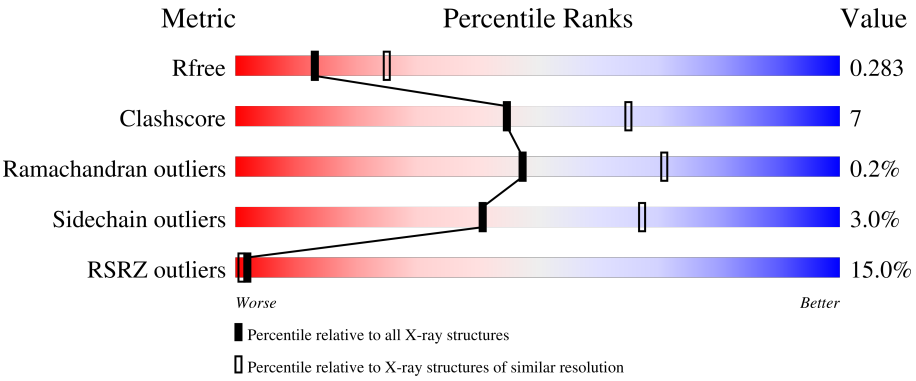
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	88% · · 7%
1	B	353	% 87% 7% 7%
1	C	353	15% 77% 15% · 7%
1	D	353	40% 70% 17% · · 9%
2	a	243	· 97%

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Mol	Chain	Length	Quality of chain
2	b	243	97%
2	c	243	97%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10746 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Isoform 2 of C-terminal-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2569	1610	464	482	13			
1	B	330	Total	C	N	O	S	0	0	0
			2569	1610	464	482	13			
1	C	330	Total	C	N	O	S	0	0	0
			2569	1610	464	482	13			
1	D	320	Total	C	N	O	S	0	0	0
			2494	1565	450	466	13			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	HIS	-	expression tag	UNP P56545-2
A	13	HIS	-	expression tag	UNP P56545-2
A	14	HIS	-	expression tag	UNP P56545-2
A	15	HIS	-	expression tag	UNP P56545-2
A	16	HIS	-	expression tag	UNP P56545-2
A	17	HIS	-	expression tag	UNP P56545-2
A	18	SER	-	expression tag	UNP P56545-2
A	19	ALA	-	expression tag	UNP P56545-2
A	20	GLY	-	expression tag	UNP P56545-2
A	21	LEU	-	expression tag	UNP P56545-2
A	22	GLU	-	expression tag	UNP P56545-2
A	23	VAL	-	expression tag	UNP P56545-2
A	24	LEU	-	expression tag	UNP P56545-2
A	25	PHE	-	expression tag	UNP P56545-2
A	26	GLN	-	expression tag	UNP P56545-2
A	27	GLY	-	expression tag	UNP P56545-2
A	28	PRO	-	expression tag	UNP P56545-2
A	29	MET	-	expression tag	UNP P56545-2
A	30	ASP	-	expression tag	UNP P56545-2
B	12	HIS	-	expression tag	UNP P56545-2
B	13	HIS	-	expression tag	UNP P56545-2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	HIS	-	expression tag	UNP P56545-2
B	15	HIS	-	expression tag	UNP P56545-2
B	16	HIS	-	expression tag	UNP P56545-2
B	17	HIS	-	expression tag	UNP P56545-2
B	18	SER	-	expression tag	UNP P56545-2
B	19	ALA	-	expression tag	UNP P56545-2
B	20	GLY	-	expression tag	UNP P56545-2
B	21	LEU	-	expression tag	UNP P56545-2
B	22	GLU	-	expression tag	UNP P56545-2
B	23	VAL	-	expression tag	UNP P56545-2
B	24	LEU	-	expression tag	UNP P56545-2
B	25	PHE	-	expression tag	UNP P56545-2
B	26	GLN	-	expression tag	UNP P56545-2
B	27	GLY	-	expression tag	UNP P56545-2
B	28	PRO	-	expression tag	UNP P56545-2
B	29	MET	-	expression tag	UNP P56545-2
B	30	ASP	-	expression tag	UNP P56545-2
C	12	HIS	-	expression tag	UNP P56545-2
C	13	HIS	-	expression tag	UNP P56545-2
C	14	HIS	-	expression tag	UNP P56545-2
C	15	HIS	-	expression tag	UNP P56545-2
C	16	HIS	-	expression tag	UNP P56545-2
C	17	HIS	-	expression tag	UNP P56545-2
C	18	SER	-	expression tag	UNP P56545-2
C	19	ALA	-	expression tag	UNP P56545-2
C	20	GLY	-	expression tag	UNP P56545-2
C	21	LEU	-	expression tag	UNP P56545-2
C	22	GLU	-	expression tag	UNP P56545-2
C	23	VAL	-	expression tag	UNP P56545-2
C	24	LEU	-	expression tag	UNP P56545-2
C	25	PHE	-	expression tag	UNP P56545-2
C	26	GLN	-	expression tag	UNP P56545-2
C	27	GLY	-	expression tag	UNP P56545-2
C	28	PRO	-	expression tag	UNP P56545-2
C	29	MET	-	expression tag	UNP P56545-2
C	30	ASP	-	expression tag	UNP P56545-2
D	12	HIS	-	expression tag	UNP P56545-2
D	13	HIS	-	expression tag	UNP P56545-2
D	14	HIS	-	expression tag	UNP P56545-2
D	15	HIS	-	expression tag	UNP P56545-2
D	16	HIS	-	expression tag	UNP P56545-2
D	17	HIS	-	expression tag	UNP P56545-2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	18	SER	-	expression tag	UNP P56545-2
D	19	ALA	-	expression tag	UNP P56545-2
D	20	GLY	-	expression tag	UNP P56545-2
D	21	LEU	-	expression tag	UNP P56545-2
D	22	GLU	-	expression tag	UNP P56545-2
D	23	VAL	-	expression tag	UNP P56545-2
D	24	LEU	-	expression tag	UNP P56545-2
D	25	PHE	-	expression tag	UNP P56545-2
D	26	GLN	-	expression tag	UNP P56545-2
D	27	GLY	-	expression tag	UNP P56545-2
D	28	PRO	-	expression tag	UNP P56545-2
D	29	MET	-	expression tag	UNP P56545-2
D	30	ASP	-	expression tag	UNP P56545-2

- Molecule 2 is a protein called Retinoic acid-induced protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	7	Total	C	N	O	S	0	0	0
			52	32	7	12	1			
2	b	7	Total	C	N	O	S	0	0	0
			52	32	7	12	1			
2	c	7	Total	C	N	O	S	0	0	0
			52	32	7	12	1			

There are 246 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	223	HIS	-	expression tag	UNP Q9Y5P3
a	224	HIS	-	expression tag	UNP Q9Y5P3
a	225	HIS	-	expression tag	UNP Q9Y5P3
a	226	HIS	-	expression tag	UNP Q9Y5P3
a	227	HIS	-	expression tag	UNP Q9Y5P3
a	228	HIS	-	expression tag	UNP Q9Y5P3
a	229	PRO	-	expression tag	UNP Q9Y5P3
a	230	MET	-	expression tag	UNP Q9Y5P3
a	231	LYS	-	expression tag	UNP Q9Y5P3
a	232	GLN	-	expression tag	UNP Q9Y5P3
a	233	TYR	-	expression tag	UNP Q9Y5P3
a	234	LYS	-	expression tag	UNP Q9Y5P3
a	235	LEU	-	expression tag	UNP Q9Y5P3
a	236	ILE	-	expression tag	UNP Q9Y5P3
a	237	LEU	-	expression tag	UNP Q9Y5P3

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Chain	Residue	Modelled	Actual	Comment	Reference
a	238	ASN	-	expression tag	UNP Q9Y5P3
a	239	GLY	-	expression tag	UNP Q9Y5P3
a	240	LYS	-	expression tag	UNP Q9Y5P3
a	241	THR	-	expression tag	UNP Q9Y5P3
a	242	LEU	-	expression tag	UNP Q9Y5P3
a	243	LYS	-	expression tag	UNP Q9Y5P3
a	244	GLY	-	expression tag	UNP Q9Y5P3
a	245	GLU	-	expression tag	UNP Q9Y5P3
a	246	THR	-	expression tag	UNP Q9Y5P3
a	247	THR	-	expression tag	UNP Q9Y5P3
a	248	THR	-	expression tag	UNP Q9Y5P3
a	249	GLU	-	expression tag	UNP Q9Y5P3
a	250	ALA	-	expression tag	UNP Q9Y5P3
a	251	VAL	-	expression tag	UNP Q9Y5P3
a	252	ASP	-	expression tag	UNP Q9Y5P3
a	253	ALA	-	expression tag	UNP Q9Y5P3
a	254	ALA	-	expression tag	UNP Q9Y5P3
a	255	THR	-	expression tag	UNP Q9Y5P3
a	256	ALA	-	expression tag	UNP Q9Y5P3
a	257	GLU	-	expression tag	UNP Q9Y5P3
a	258	LYS	-	expression tag	UNP Q9Y5P3
a	259	VAL	-	expression tag	UNP Q9Y5P3
a	260	PHE	-	expression tag	UNP Q9Y5P3
a	261	LYS	-	expression tag	UNP Q9Y5P3
a	262	GLN	-	expression tag	UNP Q9Y5P3
a	263	TYR	-	expression tag	UNP Q9Y5P3
a	264	ALA	-	expression tag	UNP Q9Y5P3
a	265	ASN	-	expression tag	UNP Q9Y5P3
a	266	ASP	-	expression tag	UNP Q9Y5P3
a	267	ASN	-	expression tag	UNP Q9Y5P3
a	268	GLY	-	expression tag	UNP Q9Y5P3
a	269	VAL	-	expression tag	UNP Q9Y5P3
a	270	ASP	-	expression tag	UNP Q9Y5P3
a	271	GLY	-	expression tag	UNP Q9Y5P3
a	272	GLU	-	expression tag	UNP Q9Y5P3
a	273	TRP	-	expression tag	UNP Q9Y5P3
a	274	THR	-	expression tag	UNP Q9Y5P3
a	275	TYR	-	expression tag	UNP Q9Y5P3
a	276	ASP	-	expression tag	UNP Q9Y5P3
a	277	ASP	-	expression tag	UNP Q9Y5P3
a	278	ALA	-	expression tag	UNP Q9Y5P3
a	279	THR	-	expression tag	UNP Q9Y5P3

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Chain	Residue	Modelled	Actual	Comment	Reference
a	280	LYS	-	expression tag	UNP Q9Y5P3
a	281	THR	-	expression tag	UNP Q9Y5P3
a	282	PHE	-	expression tag	UNP Q9Y5P3
a	283	THR	-	expression tag	UNP Q9Y5P3
a	284	VAL	-	expression tag	UNP Q9Y5P3
a	285	THR	-	expression tag	UNP Q9Y5P3
a	286	GLU	-	expression tag	UNP Q9Y5P3
a	287	GLY	-	expression tag	UNP Q9Y5P3
a	288	SER	-	expression tag	UNP Q9Y5P3
a	289	GLY	-	expression tag	UNP Q9Y5P3
a	290	SER	-	expression tag	UNP Q9Y5P3
a	291	GLY	-	expression tag	UNP Q9Y5P3
a	292	SER	-	expression tag	UNP Q9Y5P3
a	293	GLU	-	expression tag	UNP Q9Y5P3
a	294	ASN	-	expression tag	UNP Q9Y5P3
a	295	LEU	-	expression tag	UNP Q9Y5P3
a	296	TYR	-	expression tag	UNP Q9Y5P3
a	297	PHE	-	expression tag	UNP Q9Y5P3
a	298	GLN	-	expression tag	UNP Q9Y5P3
a	299	GLY	-	expression tag	UNP Q9Y5P3
a	300	ALA	-	expression tag	UNP Q9Y5P3
a	301	MET	-	expression tag	UNP Q9Y5P3
a	302	ASP	-	expression tag	UNP Q9Y5P3
a	345	ALA	LEU	conflict	UNP Q9Y5P3
a	346	ALA	SER	conflict	UNP Q9Y5P3
b	223	HIS	-	expression tag	UNP Q9Y5P3
b	224	HIS	-	expression tag	UNP Q9Y5P3
b	225	HIS	-	expression tag	UNP Q9Y5P3
b	226	HIS	-	expression tag	UNP Q9Y5P3
b	227	HIS	-	expression tag	UNP Q9Y5P3
b	228	HIS	-	expression tag	UNP Q9Y5P3
b	229	PRO	-	expression tag	UNP Q9Y5P3
b	230	MET	-	expression tag	UNP Q9Y5P3
b	231	LYS	-	expression tag	UNP Q9Y5P3
b	232	GLN	-	expression tag	UNP Q9Y5P3
b	233	TYR	-	expression tag	UNP Q9Y5P3
b	234	LYS	-	expression tag	UNP Q9Y5P3
b	235	LEU	-	expression tag	UNP Q9Y5P3
b	236	ILE	-	expression tag	UNP Q9Y5P3
b	237	LEU	-	expression tag	UNP Q9Y5P3
b	238	ASN	-	expression tag	UNP Q9Y5P3
b	239	GLY	-	expression tag	UNP Q9Y5P3

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Chain	Residue	Modelled	Actual	Comment	Reference
b	240	LYS	-	expression tag	UNP Q9Y5P3
b	241	THR	-	expression tag	UNP Q9Y5P3
b	242	LEU	-	expression tag	UNP Q9Y5P3
b	243	LYS	-	expression tag	UNP Q9Y5P3
b	244	GLY	-	expression tag	UNP Q9Y5P3
b	245	GLU	-	expression tag	UNP Q9Y5P3
b	246	THR	-	expression tag	UNP Q9Y5P3
b	247	THR	-	expression tag	UNP Q9Y5P3
b	248	THR	-	expression tag	UNP Q9Y5P3
b	249	GLU	-	expression tag	UNP Q9Y5P3
b	250	ALA	-	expression tag	UNP Q9Y5P3
b	251	VAL	-	expression tag	UNP Q9Y5P3
b	252	ASP	-	expression tag	UNP Q9Y5P3
b	253	ALA	-	expression tag	UNP Q9Y5P3
b	254	ALA	-	expression tag	UNP Q9Y5P3
b	255	THR	-	expression tag	UNP Q9Y5P3
b	256	ALA	-	expression tag	UNP Q9Y5P3
b	257	GLU	-	expression tag	UNP Q9Y5P3
b	258	LYS	-	expression tag	UNP Q9Y5P3
b	259	VAL	-	expression tag	UNP Q9Y5P3
b	260	PHE	-	expression tag	UNP Q9Y5P3
b	261	LYS	-	expression tag	UNP Q9Y5P3
b	262	GLN	-	expression tag	UNP Q9Y5P3
b	263	TYR	-	expression tag	UNP Q9Y5P3
b	264	ALA	-	expression tag	UNP Q9Y5P3
b	265	ASN	-	expression tag	UNP Q9Y5P3
b	266	ASP	-	expression tag	UNP Q9Y5P3
b	267	ASN	-	expression tag	UNP Q9Y5P3
b	268	GLY	-	expression tag	UNP Q9Y5P3
b	269	VAL	-	expression tag	UNP Q9Y5P3
b	270	ASP	-	expression tag	UNP Q9Y5P3
b	271	GLY	-	expression tag	UNP Q9Y5P3
b	272	GLU	-	expression tag	UNP Q9Y5P3
b	273	TRP	-	expression tag	UNP Q9Y5P3
b	274	THR	-	expression tag	UNP Q9Y5P3
b	275	TYR	-	expression tag	UNP Q9Y5P3
b	276	ASP	-	expression tag	UNP Q9Y5P3
b	277	ASP	-	expression tag	UNP Q9Y5P3
b	278	ALA	-	expression tag	UNP Q9Y5P3
b	279	THR	-	expression tag	UNP Q9Y5P3
b	280	LYS	-	expression tag	UNP Q9Y5P3
b	281	THR	-	expression tag	UNP Q9Y5P3

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Chain	Residue	Modelled	Actual	Comment	Reference
b	282	PHE	-	expression tag	UNP Q9Y5P3
b	283	THR	-	expression tag	UNP Q9Y5P3
b	284	VAL	-	expression tag	UNP Q9Y5P3
b	285	THR	-	expression tag	UNP Q9Y5P3
b	286	GLU	-	expression tag	UNP Q9Y5P3
b	287	GLY	-	expression tag	UNP Q9Y5P3
b	288	SER	-	expression tag	UNP Q9Y5P3
b	289	GLY	-	expression tag	UNP Q9Y5P3
b	290	SER	-	expression tag	UNP Q9Y5P3
b	291	GLY	-	expression tag	UNP Q9Y5P3
b	292	SER	-	expression tag	UNP Q9Y5P3
b	293	GLU	-	expression tag	UNP Q9Y5P3
b	294	ASN	-	expression tag	UNP Q9Y5P3
b	295	LEU	-	expression tag	UNP Q9Y5P3
b	296	TYR	-	expression tag	UNP Q9Y5P3
b	297	PHE	-	expression tag	UNP Q9Y5P3
b	298	GLN	-	expression tag	UNP Q9Y5P3
b	299	GLY	-	expression tag	UNP Q9Y5P3
b	300	ALA	-	expression tag	UNP Q9Y5P3
b	301	MET	-	expression tag	UNP Q9Y5P3
b	302	ASP	-	expression tag	UNP Q9Y5P3
b	345	ALA	LEU	conflict	UNP Q9Y5P3
b	346	ALA	SER	conflict	UNP Q9Y5P3
c	223	HIS	-	expression tag	UNP Q9Y5P3
c	224	HIS	-	expression tag	UNP Q9Y5P3
c	225	HIS	-	expression tag	UNP Q9Y5P3
c	226	HIS	-	expression tag	UNP Q9Y5P3
c	227	HIS	-	expression tag	UNP Q9Y5P3
c	228	HIS	-	expression tag	UNP Q9Y5P3
c	229	PRO	-	expression tag	UNP Q9Y5P3
c	230	MET	-	expression tag	UNP Q9Y5P3
c	231	LYS	-	expression tag	UNP Q9Y5P3
c	232	GLN	-	expression tag	UNP Q9Y5P3
c	233	TYR	-	expression tag	UNP Q9Y5P3
c	234	LYS	-	expression tag	UNP Q9Y5P3
c	235	LEU	-	expression tag	UNP Q9Y5P3
c	236	ILE	-	expression tag	UNP Q9Y5P3
c	237	LEU	-	expression tag	UNP Q9Y5P3
c	238	ASN	-	expression tag	UNP Q9Y5P3
c	239	GLY	-	expression tag	UNP Q9Y5P3
c	240	LYS	-	expression tag	UNP Q9Y5P3
c	241	THR	-	expression tag	UNP Q9Y5P3

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Chain	Residue	Modelled	Actual	Comment	Reference
c	242	LEU	-	expression tag	UNP Q9Y5P3
c	243	LYS	-	expression tag	UNP Q9Y5P3
c	244	GLY	-	expression tag	UNP Q9Y5P3
c	245	GLU	-	expression tag	UNP Q9Y5P3
c	246	THR	-	expression tag	UNP Q9Y5P3
c	247	THR	-	expression tag	UNP Q9Y5P3
c	248	THR	-	expression tag	UNP Q9Y5P3
c	249	GLU	-	expression tag	UNP Q9Y5P3
c	250	ALA	-	expression tag	UNP Q9Y5P3
c	251	VAL	-	expression tag	UNP Q9Y5P3
c	252	ASP	-	expression tag	UNP Q9Y5P3
c	253	ALA	-	expression tag	UNP Q9Y5P3
c	254	ALA	-	expression tag	UNP Q9Y5P3
c	255	THR	-	expression tag	UNP Q9Y5P3
c	256	ALA	-	expression tag	UNP Q9Y5P3
c	257	GLU	-	expression tag	UNP Q9Y5P3
c	258	LYS	-	expression tag	UNP Q9Y5P3
c	259	VAL	-	expression tag	UNP Q9Y5P3
c	260	PHE	-	expression tag	UNP Q9Y5P3
c	261	LYS	-	expression tag	UNP Q9Y5P3
c	262	GLN	-	expression tag	UNP Q9Y5P3
c	263	TYR	-	expression tag	UNP Q9Y5P3
c	264	ALA	-	expression tag	UNP Q9Y5P3
c	265	ASN	-	expression tag	UNP Q9Y5P3
c	266	ASP	-	expression tag	UNP Q9Y5P3
c	267	ASN	-	expression tag	UNP Q9Y5P3
c	268	GLY	-	expression tag	UNP Q9Y5P3
c	269	VAL	-	expression tag	UNP Q9Y5P3
c	270	ASP	-	expression tag	UNP Q9Y5P3
c	271	GLY	-	expression tag	UNP Q9Y5P3
c	272	GLU	-	expression tag	UNP Q9Y5P3
c	273	TRP	-	expression tag	UNP Q9Y5P3
c	274	THR	-	expression tag	UNP Q9Y5P3
c	275	TYR	-	expression tag	UNP Q9Y5P3
c	276	ASP	-	expression tag	UNP Q9Y5P3
c	277	ASP	-	expression tag	UNP Q9Y5P3
c	278	ALA	-	expression tag	UNP Q9Y5P3
c	279	THR	-	expression tag	UNP Q9Y5P3
c	280	LYS	-	expression tag	UNP Q9Y5P3
c	281	THR	-	expression tag	UNP Q9Y5P3
c	282	PHE	-	expression tag	UNP Q9Y5P3
c	283	THR	-	expression tag	UNP Q9Y5P3

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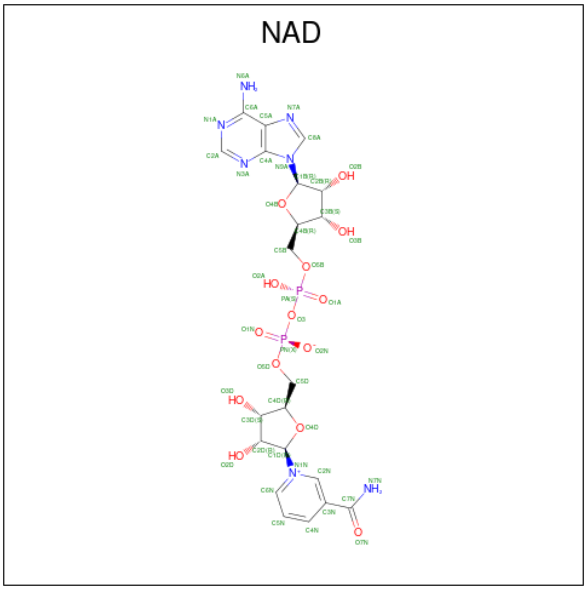
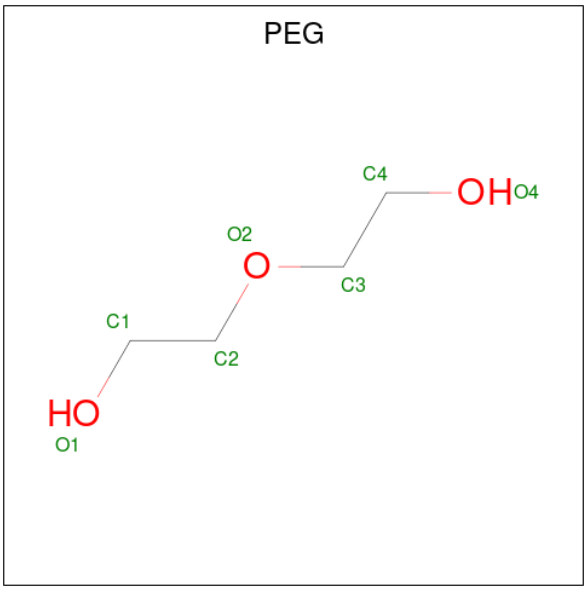
Chain	Residue	Modelled	Actual	Comment	Reference
c	284	VAL	-	expression tag	UNP Q9Y5P3
c	285	THR	-	expression tag	UNP Q9Y5P3
c	286	GLU	-	expression tag	UNP Q9Y5P3
c	287	GLY	-	expression tag	UNP Q9Y5P3
c	288	SER	-	expression tag	UNP Q9Y5P3
c	289	GLY	-	expression tag	UNP Q9Y5P3
c	290	SER	-	expression tag	UNP Q9Y5P3
c	291	GLY	-	expression tag	UNP Q9Y5P3
c	292	SER	-	expression tag	UNP Q9Y5P3
c	293	GLU	-	expression tag	UNP Q9Y5P3
c	294	ASN	-	expression tag	UNP Q9Y5P3
c	295	LEU	-	expression tag	UNP Q9Y5P3
c	296	TYR	-	expression tag	UNP Q9Y5P3
c	297	PHE	-	expression tag	UNP Q9Y5P3
c	298	GLN	-	expression tag	UNP Q9Y5P3
c	299	GLY	-	expression tag	UNP Q9Y5P3
c	300	ALA	-	expression tag	UNP Q9Y5P3
c	301	MET	-	expression tag	UNP Q9Y5P3
c	302	ASP	-	expression tag	UNP Q9Y5P3
c	345	ALA	LEU	conflict	UNP Q9Y5P3
c	346	ALA	SER	conflict	UNP Q9Y5P3

- Molecule 3 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					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O		0	0
			7	4	3			

- Molecule 5 is water.

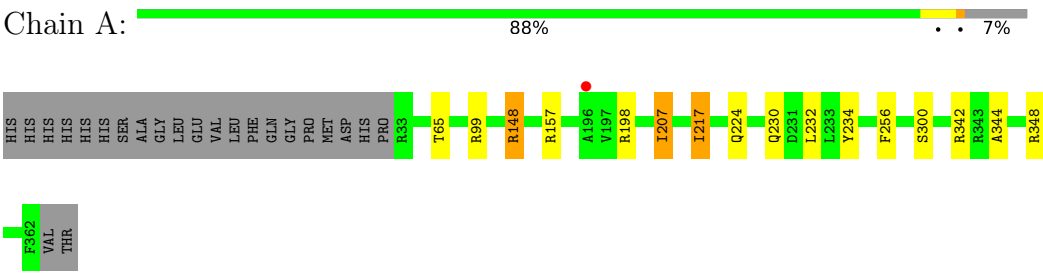
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	70	Total	O		0	0
			70	70			
5	B	98	Total	O		0	0
			98	98			
5	C	17	Total	O		0	0
			17	17			
5	D	21	Total	O		0	0
			21	21			

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

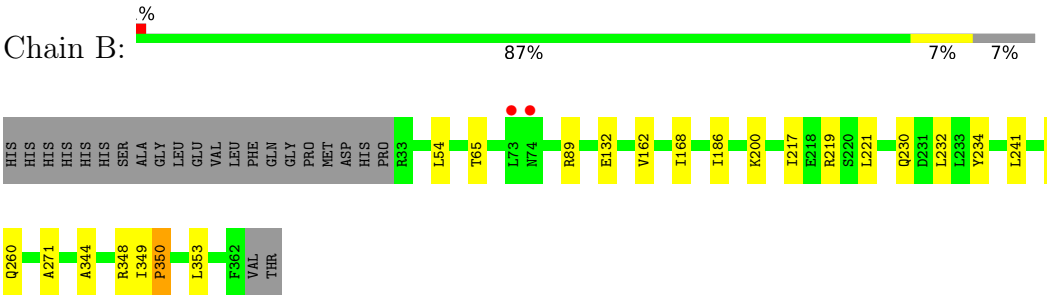
• Molecule 1: Isoform 2 of C-terminal-binding protein 2

Chain A:



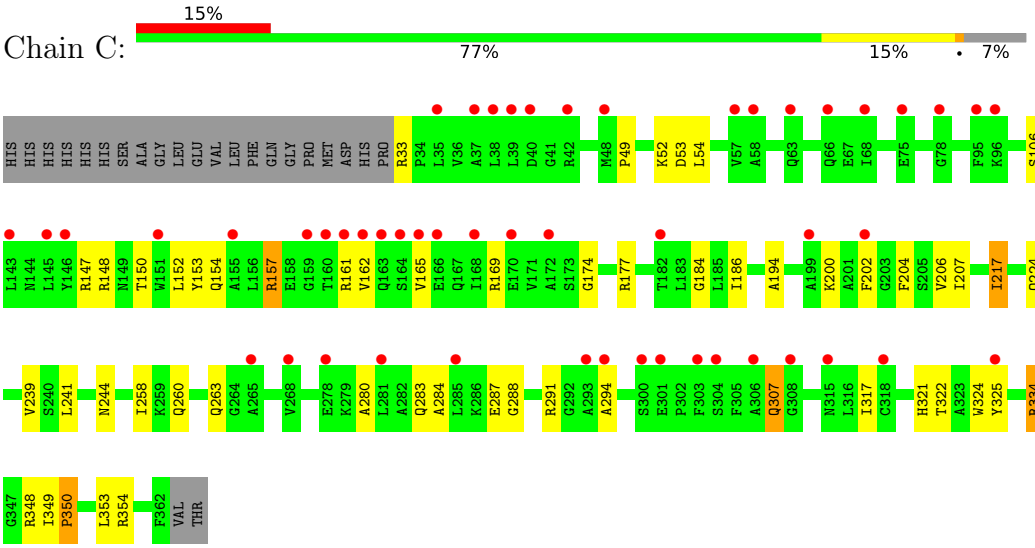
• Molecule 1: Isoform 2 of C-terminal-binding protein 2

Chain B:



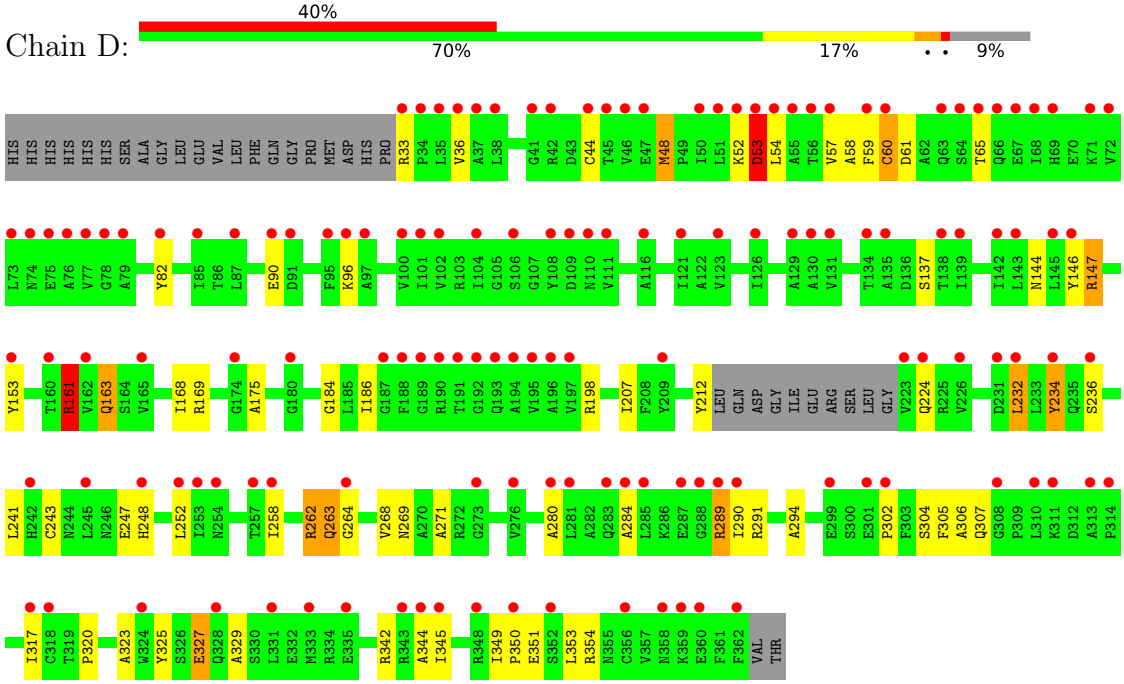
• Molecule 1: Isoform 2 of C-terminal-binding protein 2

Chain C:



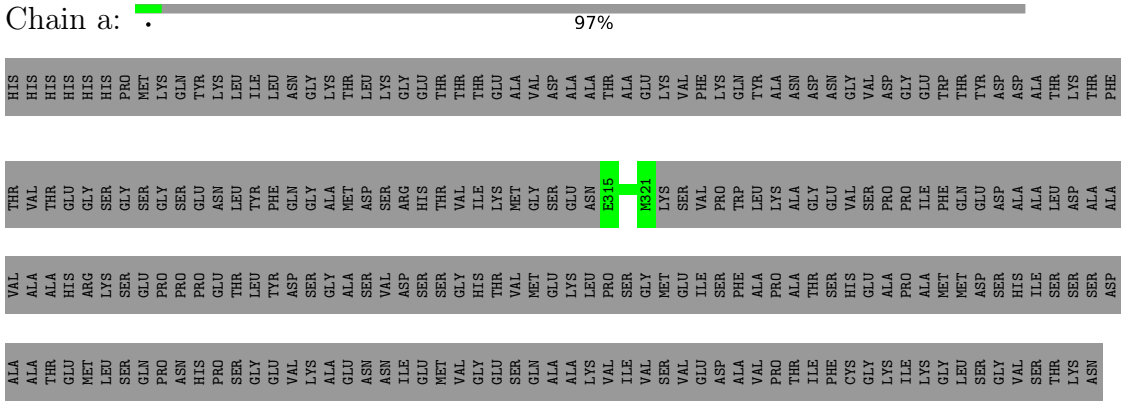
• Molecule 1: Isoform 2 of C-terminal-binding protein 2

Chain D:



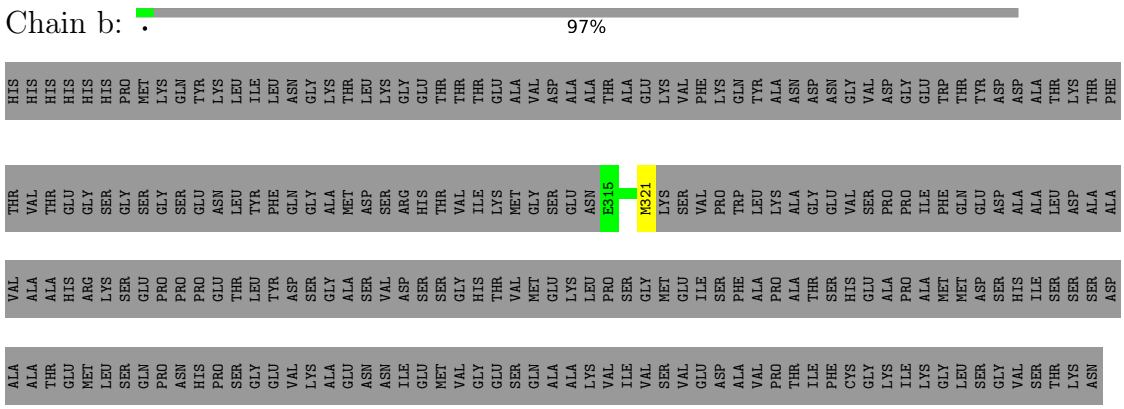
• Molecule 2: Retinoic acid-induced protein 2

Chain a:



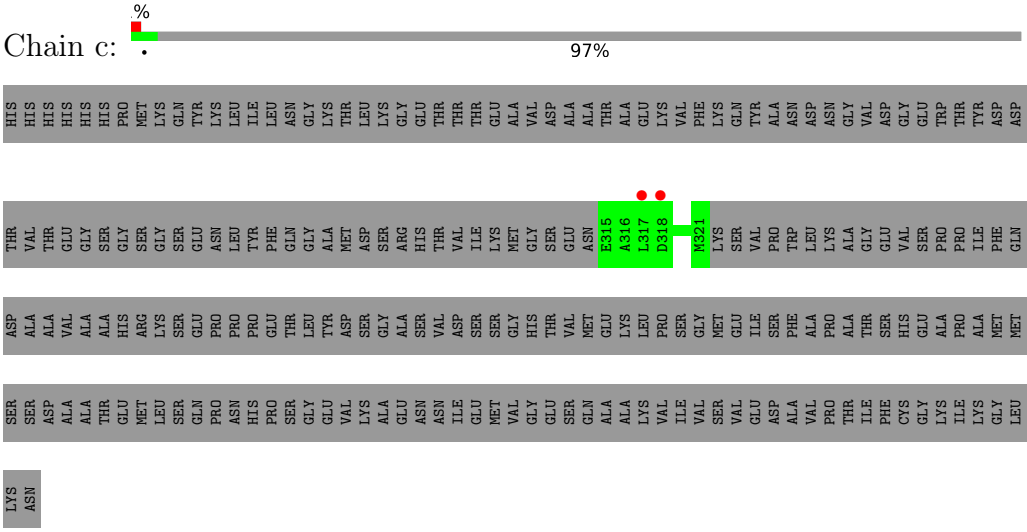
• Molecule 2: Retinoic acid-induced protein 2

Chain b:



• Molecule 2: Retinoic acid-induced protein 2

Chain c:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.65Å 126.65Å 357.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.87 – 2.60 49.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.87-2.60) 99.9 (49.82-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.228 , 0.283 0.228 , 0.283	Depositor DCC
R_{free} test set	2633 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10746	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PEG

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	0.52	0/2611	0.88	2/3533 (0.1%)
1	B	0.55	1/2611 (0.0%)	0.88	1/3533 (0.0%)
1	C	0.44	0/2611	0.85	1/3533 (0.0%)
1	D	0.42	0/2535	0.85	4/3430 (0.1%)
2	a	0.57	0/51	0.77	0/67
2	b	0.54	0/51	0.75	0/67
2	c	0.57	0/51	0.82	0/67
All	All	0.49	1/10521 (0.0%)	0.87	8/14230 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
1	D	0	3
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	GLU	CD-OE2	5.51	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	GLN	CB-CG-CD	7.67	131.54	111.60
1	A	342	ARG	CG-CD-NE	-6.67	97.79	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	327	GLU	CB-CA-C	6.06	122.52	110.40
1	D	53	ASP	CB-CA-C	5.36	121.11	110.40
1	D	161	ARG	CB-CG-CD	-5.29	97.84	111.60
1	D	234	TYR	CB-CA-C	5.14	120.68	110.40
1	C	334	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	234	TYR	CB-CG-CD1	5.06	124.04	121.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	348	ARG	Sidechain
1	C	157	ARG	Sidechain
1	C	204	PHE	Peptide
1	C	354	ARG	Sidechain
1	D	289	ARG	Sidechain
1	D	33	ARG	Sidechain
1	D	354	ARG	Sidechain

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	2569	0	2566	13	0
1	B	2569	0	2566	13	0
1	C	2569	0	2566	65	0
1	D	2494	0	2490	68	0
2	a	52	0	50	0	0
2	b	52	0	50	0	0
2	c	52	0	50	0	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	8	0
3	D	44	0	26	5	0
4	D	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	70	0	0	1	0
5	B	98	0	0	5	0
5	C	17	0	0	1	0
5	D	21	0	0	2	0
All	All	10746	0	10452	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (134) 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:D:44:CYS:O	1:D:48:MET:HG2	1.36	1.24
1:D:147:ARG:HH21	1:D:147:ARG:HG3	1.26	1.00
1:D:44:CYS:O	1:D:48:MET:CG	2.09	0.99
1:D:147:ARG:HG3	1:D:147:ARG:NH2	1.76	0.95
1:A:217:ILE:HD12	1:A:217:ILE:H	1.42	0.84
1:C:217:ILE:H	1:C:217:ILE:HD12	1.40	0.84
1:C:148:ARG:HH11	1:C:174:GLY:HA3	1.43	0.82
1:D:263:GLN:OE1	1:D:264:GLY:N	2.13	0.81
1:C:161:ARG:HH11	1:D:304:SER:HB2	1.45	0.81
1:C:258:ILE:HD12	1:C:280:ALA:HB1	1.63	0.81
1:C:150:THR:CG2	1:D:153:TYR:CD2	2.65	0.79
1:B:250:HIS:CD2	5:B:583:HOH:O	2.36	0.78
1:C:165:VAL:HG21	1:D:82:TYR:CD2	2.19	0.77
1:D:147:ARG:HH21	1:D:147:ARG:CG	1.97	0.77
1:C:54:LEU:HD21	1:C:346:THR:CG2	2.18	0.74
1:D:350:PRO:HD2	1:D:351:GLU:OE1	1.86	0.74
1:C:258:ILE:HD12	1:C:280:ALA:CB	2.17	0.74
1:C:169:ARG:HE	1:D:325:TYR:HE1	1.34	0.73
1:C:148:ARG:NH1	1:C:174:GLY:HA3	2.03	0.73
1:C:307:GLN:HA	1:C:307:GLN:HE21	1.58	0.68
1:B:250:HIS:HD2	5:B:583:HOH:O	1.73	0.67
1:A:217:ILE:H	1:A:217:ILE:CD1	2.08	0.67
1:D:59:PHE:O	1:D:60:CYS:SG	2.51	0.66
1:C:322:THR:O	1:D:147:ARG:NH1	2.29	0.65
1:C:217:ILE:HD12	1:C:217:ILE:N	2.12	0.65
1:D:186:ILE:HB	1:D:241:LEU:HD23	1.77	0.64
1:D:241:LEU:HB2	1:D:269:ASN:OD1	1.97	0.64
1:C:217:ILE:H	1:C:217:ILE:CD1	2.09	0.64
1:C:324:TRP:HD1	3:C:401:NAD:N7N	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:TRP:HB3	3:C:401:NAD:H71N	1.63	0.63
1:C:147:ARG:NH1	1:D:323:ALA:O	2.33	0.62
1:A:217:ILE:HD12	1:A:217:ILE:N	2.12	0.61
1:C:244:ASN:HA	3:C:401:NAD:O3D	2.01	0.61
1:D:58:ALA:O	1:D:59:PHE:HB2	2.01	0.61
1:C:54:LEU:HD21	1:C:346:THR:HG22	1.83	0.60
1:C:177:ARG:HH11	1:D:329:ALA:HB2	1.67	0.60
1:D:247:GLU:H	1:D:247:GLU:CD	2.05	0.60
1:D:258:ILE:HG22	1:D:289:ARG:HH12	1.67	0.60
1:D:306:ALA:O	1:D:307:GLN:HG3	2.02	0.59
1:C:33:ARG:HH22	1:C:53:ASP:HA	1.68	0.59
1:C:154:GLN:HG3	5:D:521:HOH:O	2.03	0.58
1:D:280:ALA:HB3	5:D:505:HOH:O	2.04	0.57
1:D:258:ILE:CG2	1:D:289:ARG:HH12	2.17	0.57
1:C:162:VAL:O	1:D:302:PRO:HB3	2.04	0.57
1:B:247:GLU:H	1:B:247:GLU:CD	2.08	0.57
1:B:230:GLN:HG3	1:B:260:GLN:NE2	2.20	0.57
1:B:271:ALA:HA	3:B:401:NAD:H1D	1.85	0.57
1:C:165:VAL:HG21	1:D:82:TYR:CG	2.41	0.56
1:C:322:THR:HG22	1:D:168:ILE:HG23	1.87	0.56
1:D:243:CYS:O	3:D:401:NAD:O3D	2.23	0.56
1:C:147:ARG:NH1	1:D:137:SER:OG	2.39	0.55
1:C:324:TRP:CD1	3:C:401:NAD:N7N	2.72	0.55
1:C:148:ARG:HE	1:C:174:GLY:C	2.09	0.55
1:C:291:ARG:NH1	5:C:504:HOH:O	2.40	0.55
1:D:327:GLU:OE1	1:D:327:GLU:N	2.32	0.55
1:D:54:LEU:HD12	1:D:342:ARG:NH2	2.22	0.55
1:C:186:ILE:HB	1:C:241:LEU:HD23	1.88	0.54
1:C:325:TYR:CE1	1:D:169:ARG:HG2	2.43	0.54
1:D:212:TYR:HE2	3:D:401:NAD:C8A	2.20	0.54
1:C:147:ARG:NH2	1:D:325:TYR:O	2.32	0.54
1:D:212:TYR:HE2	3:D:401:NAD:N7A	2.06	0.54
1:B:344:ALA:HB2	1:B:353:LEU:HD21	1.89	0.53
1:C:206:VAL:O	1:C:207:ILE:HD12	2.09	0.53
1:C:263:GLN:HE21	1:C:263:GLN:HA	1.74	0.52
1:D:161:ARG:NH1	1:D:163:GLN:HB3	2.24	0.52
1:C:150:THR:HG21	1:D:153:TYR:CD2	2.44	0.52
1:A:148:ARG:HD3	5:A:514:HOH:O	2.08	0.52
1:C:157:ARG:HH21	1:D:305:PHE:HB3	1.75	0.52
1:D:186:ILE:HG21	1:D:252:LEU:HD21	1.92	0.52
1:D:236:SER:O	1:D:262:ARG:HD2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LYS:NZ	1:B:221:LEU:O	2.39	0.51
1:A:99:ARG:CZ	1:A:349:ILE:HD12	2.41	0.50
1:A:256:PHE:CE2	1:C:288:GLY:HA3	2.46	0.50
1:D:271:ALA:O	3:D:401:NAD:H2N	2.11	0.50
1:C:161:ARG:HH11	1:D:304:SER:CB	2.19	0.50
1:C:230:GLN:HG2	1:C:260:GLN:NE2	2.26	0.50
1:C:263:GLN:HA	1:C:263:GLN:NE2	2.27	0.50
1:D:344:ALA:HB2	1:D:353:LEU:HD21	1.93	0.50
1:D:36:VAL:HG21	1:D:345:ILE:HD11	1.95	0.49
1:C:324:TRP:HD1	3:C:401:NAD:H72N	1.60	0.49
1:A:207:ILE:HG13	1:A:224:GLN:HB3	1.95	0.48
1:A:344:ALA:HB2	1:A:353:LEU:HD21	1.95	0.48
1:A:256:PHE:HE2	1:C:287:GLU:O	1.98	0.47
1:C:153:TYR:HE1	1:D:305:PHE:CZ	2.32	0.47
1:C:230:GLN:HG2	1:C:260:GLN:CD	2.35	0.47
1:D:147:ARG:NH2	1:D:147:ARG:O	2.47	0.46
1:C:150:THR:HG22	1:D:153:TYR:CD2	2.50	0.46
1:C:135:ALA:HB2	1:C:194:ALA:HB3	1.98	0.46
1:C:258:ILE:HG21	1:C:284:ALA:HB2	1.98	0.46
1:A:198:ARG:HH21	1:A:198:ARG:HG3	1.81	0.46
1:C:148:ARG:HH11	1:C:174:GLY:CA	2.21	0.46
1:D:186:ILE:HG13	1:D:232:LEU:HD22	1.98	0.46
1:C:177:ARG:NH1	1:D:329:ALA:HB2	2.28	0.45
1:D:284:ALA:HB1	1:D:290:ILE:HG12	1.98	0.45
1:C:150:THR:HG22	1:D:153:TYR:CE2	2.51	0.45
1:D:161:ARG:HE	1:D:161:ARG:HB3	1.31	0.45
1:B:250:HIS:HB2	5:B:583:HOH:O	2.17	0.45
1:C:349:ILE:HA	1:C:350:PRO:HA	1.70	0.45
1:B:89:ARG:NH2	5:B:508:HOH:O	2.50	0.44
1:C:54:LEU:CD2	1:C:346:THR:CG2	2.91	0.44
3:C:401:NAD:H6N	3:C:401:NAD:H2D	1.57	0.44
1:C:294:ALA:HA	1:C:317:ILE:O	2.17	0.44
1:C:106:SER:OG	3:C:401:NAD:H6N	2.18	0.44
1:C:33:ARG:NH2	1:C:53:ASP:HA	2.30	0.43
1:C:202:PHE:CD1	1:C:202:PHE:N	2.86	0.43
1:D:236:SER:C	1:D:262:ARG:HD2	2.39	0.43
1:C:157:ARG:NH2	1:D:305:PHE:HB3	2.33	0.43
1:D:144:ASN:HB3	1:D:317:ILE:CD1	2.48	0.43
1:D:247:GLU:HG2	1:D:248:HIS:CD2	2.53	0.43
1:D:52:LYS:HB3	1:D:53:ASP:OD1	2.18	0.43
1:D:198:ARG:HG3	1:D:198:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LEU:HD22	1:D:320:PRO:HD2	2.00	0.43
1:A:349:ILE:HA	1:A:350:PRO:HA	1.72	0.43
1:D:349:ILE:HA	1:D:350:PRO:HA	1.70	0.43
1:C:49:PRO:HA	1:C:52:LYS:HE3	2.01	0.43
1:A:207:ILE:HA	1:A:224:GLN:O	2.19	0.43
1:B:186:ILE:HB	1:B:241:LEU:HD23	2.00	0.43
1:D:268:VAL:HG22	1:D:294:ALA:HB3	2.00	0.43
1:C:161:ARG:NH1	1:D:304:SER:HB2	2.23	0.42
1:C:184:GLY:O	1:C:239:VAL:HA	2.18	0.42
1:D:212:TYR:CE2	3:D:401:NAD:C8A	3.02	0.42
1:D:264:GLY:HA2	1:D:291:ARG:HB2	2.02	0.42
1:D:57:VAL:HG22	1:D:58:ALA:H	1.84	0.42
1:A:217:ILE:CD1	1:A:217:ILE:N	2.79	0.42
1:B:162:VAL:HG12	1:B:168:ILE:HG13	2.02	0.42
1:D:184:GLY:HA3	1:D:236:SER:OG	2.20	0.41
1:D:207:ILE:HA	1:D:224:GLN:O	2.21	0.41
1:B:219:ARG:HD3	5:B:511:HOH:O	2.20	0.41
1:C:321:HIS:CD2	3:C:401:NAD:O7N	2.74	0.41
1:D:146:TYR:O	1:D:175:ALA:HA	2.21	0.40
1:C:207:ILE:HA	1:C:224:GLN:O	2.21	0.40
1:B:349:ILE:HA	1:B:350:PRO:HA	1.66	0.40
1:C:334:ARG:HD2	1:D:169:ARG:HH11	1.87	0.40
1:C:344:ALA:HB2	1:C:353:LEU:HD21	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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	328/353 (93%)	315 (96%)	13 (4%)	0	100	100
1	B	328/353 (93%)	314 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	328/353 (93%)	311 (95%)	17 (5%)	0	100 100
1	D	316/353 (90%)	297 (94%)	17 (5%)	2 (1%)	25 47
2	a	5/243 (2%)	5 (100%)	0	0	100 100
2	b	5/243 (2%)	4 (80%)	1 (20%)	0	100 100
2	c	5/243 (2%)	4 (80%)	1 (20%)	0	100 100
All	All	1315/2141 (61%)	1250 (95%)	63 (5%)	2 (0%)	47 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	61	ASP
1	D	60	CYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	270/290 (93%)	263 (97%)	7 (3%)	46 72
1	B	270/290 (93%)	264 (98%)	6 (2%)	52 76
1	C	270/290 (93%)	263 (97%)	7 (3%)	46 72
1	D	262/290 (90%)	250 (95%)	12 (5%)	27 51
2	a	6/199 (3%)	6 (100%)	0	100 100
2	b	6/199 (3%)	5 (83%)	1 (17%)	2 3
2	c	6/199 (3%)	6 (100%)	0	100 100
All	All	1090/1757 (62%)	1057 (97%)	33 (3%)	41 67

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	THR
1	A	207	ILE

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Mol	Chain	Res	Type
1	A	217	ILE
1	A	232	LEU
1	A	234	TYR
1	A	300	SER
1	A	350	PRO
1	B	54	LEU
1	B	65	THR
1	B	217	ILE
1	B	232	LEU
1	B	348	ARG
1	B	350	PRO
1	C	200	LYS
1	C	217	ILE
1	C	232	LEU
1	C	283	GLN
1	C	307	GLN
1	C	348	ARG
1	C	350	PRO
1	D	48	MET
1	D	53	ASP
1	D	65	THR
1	D	90	GLU
1	D	96	LYS
1	D	147	ARG
1	D	161	ARG
1	D	163	GLN
1	D	232	LEU
1	D	234	TYR
1	D	262	ARG
1	D	263	GLN
2	b	321	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	263	GLN
1	B	230	GLN
1	B	260	GLN
1	C	149	ASN
1	C	263	GLN
1	C	307	GLN

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Mol	Chain	Res	Type
1	D	141	HIS
1	D	248	HIS
1	D	250	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

5 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	$\#\|Z\| > 2$
3	NAD	D	401	-	42,48,48	0.88	1 (2%)	50,73,73	1.60	8 (16%)
3	NAD	C	401	-	42,48,48	0.79	1 (2%)	50,73,73	1.18	5 (10%)
3	NAD	A	401	-	42,48,48	0.85	1 (2%)	50,73,73	1.12	5 (10%)
3	NAD	B	401	-	42,48,48	0.82	2 (4%)	50,73,73	0.84	0
4	PEG	D	402	-	6,6,6	0.41	0	5,5,5	0.34	0

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	NAD	D	401	-	-	12/26/62/62	0/5/5/5
3	NAD	C	401	-	-	5/26/62/62	0/5/5/5
3	NAD	A	401	-	-	2/26/62/62	0/5/5/5
3	NAD	B	401	-	-	2/26/62/62	0/5/5/5
4	PEG	D	402	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NAD	C2N-N1N	3.76	1.39	1.35
3	A	401	NAD	C2N-N1N	3.46	1.39	1.35
3	B	401	NAD	C2N-N1N	2.92	1.38	1.35
3	C	401	NAD	C2N-N1N	2.65	1.38	1.35
3	B	401	NAD	C8A-N7A	-2.31	1.30	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	NAD	O3D-C3D-C4D	-5.97	93.80	111.05
3	C	401	NAD	O4B-C1B-C2B	-4.08	100.96	106.93
3	D	401	NAD	C6N-N1N-C2N	-3.58	118.71	121.97
3	D	401	NAD	O4B-C1B-C2B	-3.18	102.28	106.93
3	D	401	NAD	O2B-C2B-C1B	2.98	121.85	110.85
3	D	401	NAD	PN-O3-PA	2.97	143.00	132.83
3	A	401	NAD	O4B-C1B-C2B	-2.77	102.88	106.93
3	C	401	NAD	C6N-N1N-C2N	-2.77	119.45	121.97
3	D	401	NAD	O2D-C2D-C1D	2.63	120.56	110.85
3	D	401	NAD	C5A-C6A-N6A	2.60	124.30	120.35
3	D	401	NAD	O4D-C1D-C2D	-2.38	103.45	106.93
3	C	401	NAD	O2B-C2B-C1B	-2.37	102.09	110.85
3	C	401	NAD	PN-O3-PA	-2.34	124.81	132.83
3	A	401	NAD	C3N-C2N-N1N	2.25	122.63	120.43
3	A	401	NAD	O2A-PA-O1A	2.14	122.81	112.24
3	C	401	NAD	C5A-C6A-N6A	2.12	123.57	120.35
3	A	401	NAD	C4A-C5A-N7A	2.11	111.60	109.40
3	A	401	NAD	PN-O3-PA	-2.00	125.95	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAD	O4D-C1D-N1N-C6N
3	C	401	NAD	O4D-C1D-N1N-C2N
3	C	401	NAD	O4D-C1D-N1N-C6N
3	C	401	NAD	C2D-C1D-N1N-C2N
3	C	401	NAD	C2D-C1D-N1N-C6N
3	D	401	NAD	C5D-O5D-PN-O1N
3	D	401	NAD	O4D-C1D-N1N-C2N
3	D	401	NAD	O4D-C1D-N1N-C6N
3	D	401	NAD	C2D-C1D-N1N-C2N
3	D	401	NAD	C2D-C1D-N1N-C6N
3	D	401	NAD	C3D-C4D-C5D-O5D
3	D	401	NAD	O4D-C4D-C5D-O5D
3	A	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	O4B-C4B-C5B-O5B
3	D	401	NAD	C5D-O5D-PN-O3
3	D	401	NAD	C5D-O5D-PN-O2N
4	D	402	PEG	C1-C2-O2-C3
3	D	401	NAD	PN-O3-PA-O2A
3	D	401	NAD	PN-O3-PA-O1A
3	C	401	NAD	O4B-C4B-C5B-O5B
3	D	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	PN-O3-PA-O2A

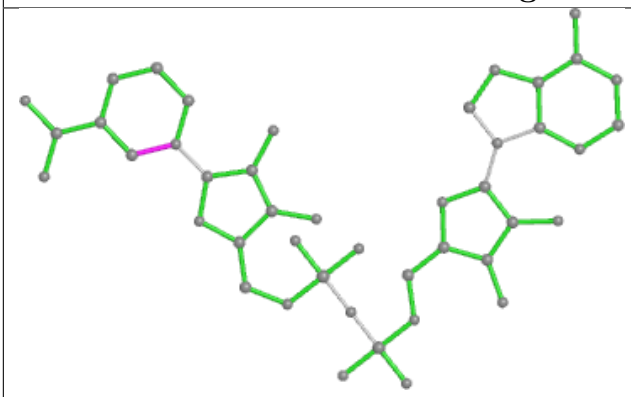
There are no ring outliers.

3 monomers are involved in 14 short contacts:

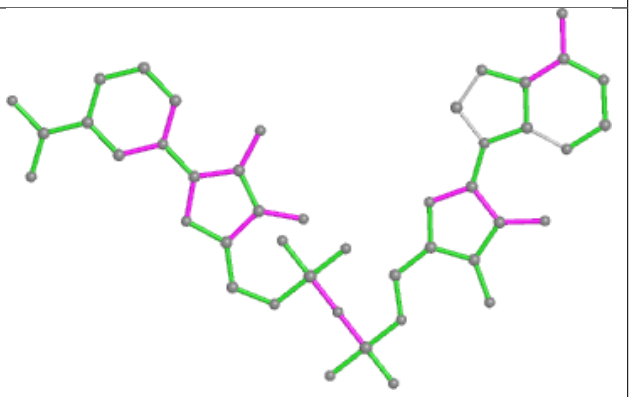
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	NAD	5	0
3	C	401	NAD	8	0
3	B	401	NAD	1	0

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.

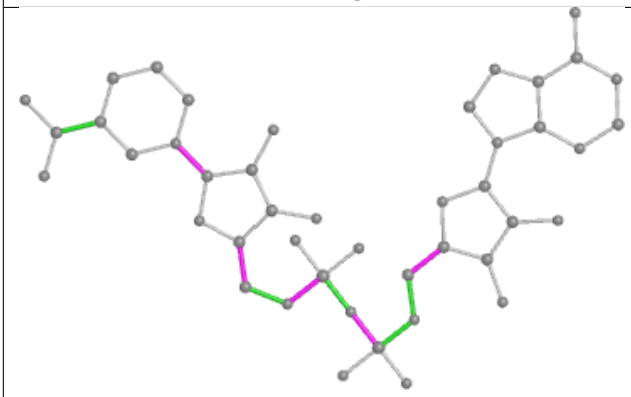
Ligand NAD D 401



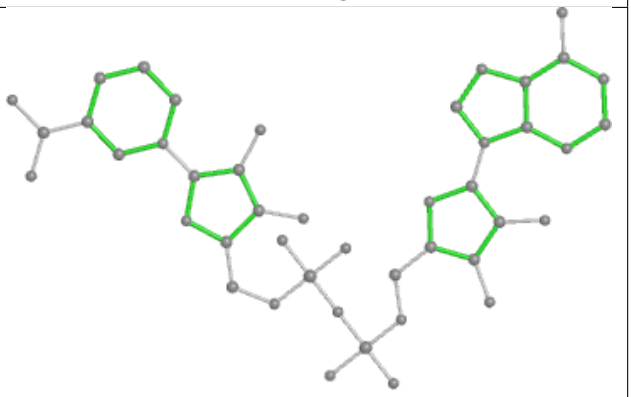
Bond lengths



Bond angles

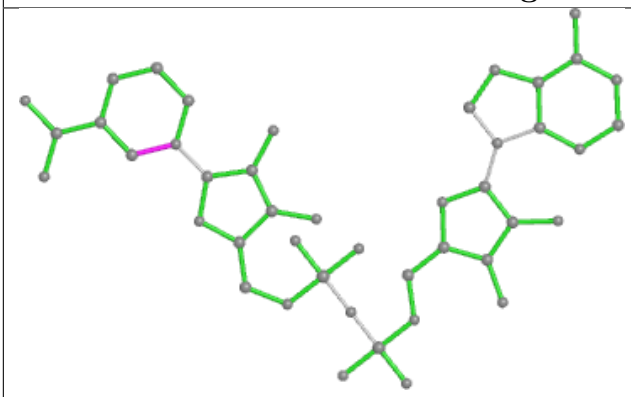


Torsions

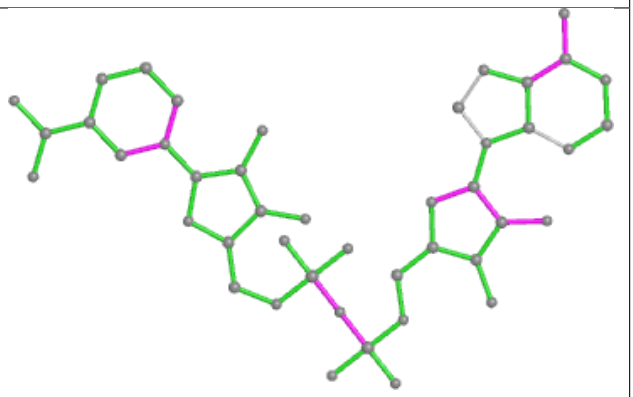


Rings

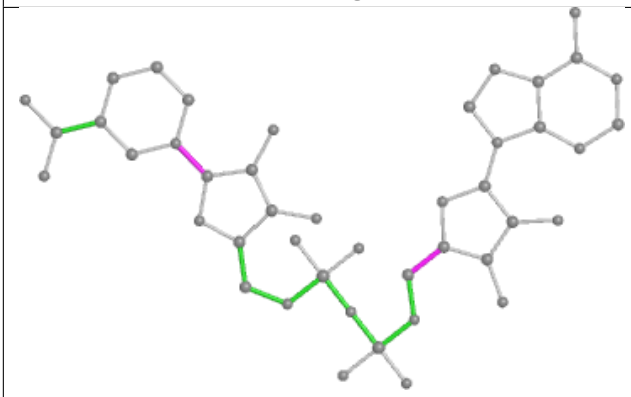
Ligand NAD C 401



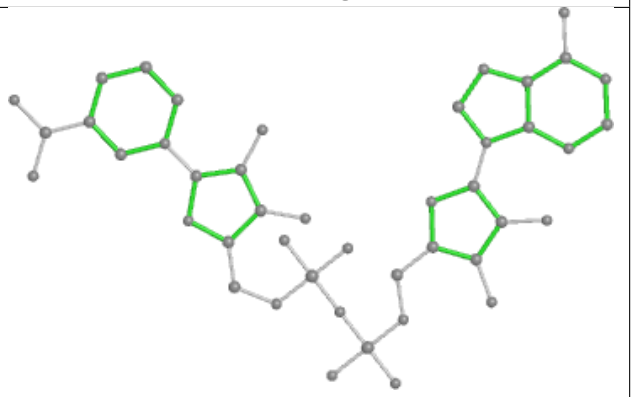
Bond lengths



Bond angles

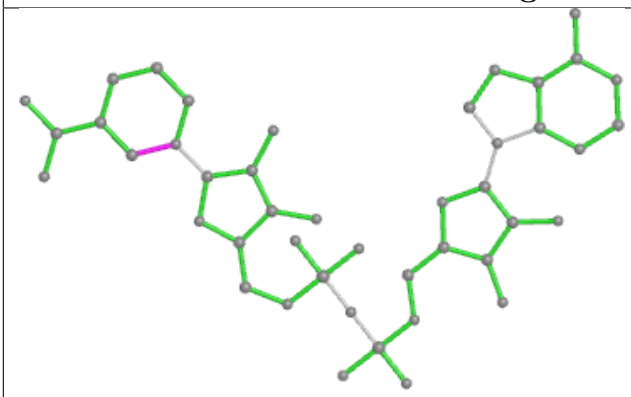


Torsions

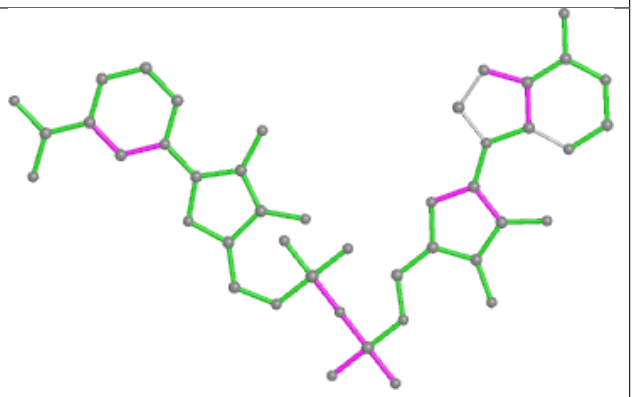


Rings

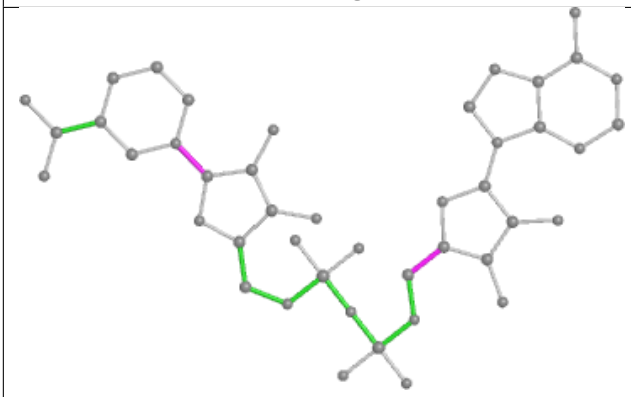
Ligand NAD A 401



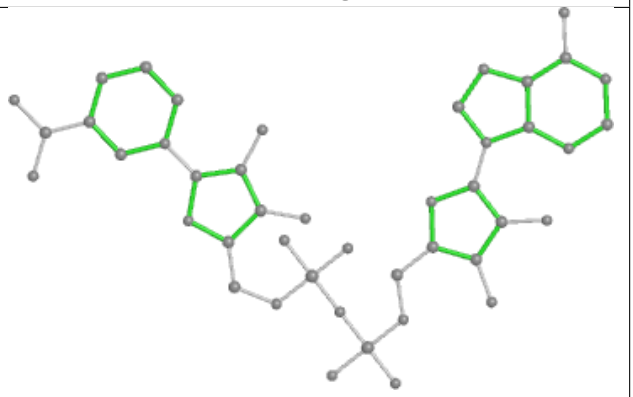
Bond lengths



Bond angles

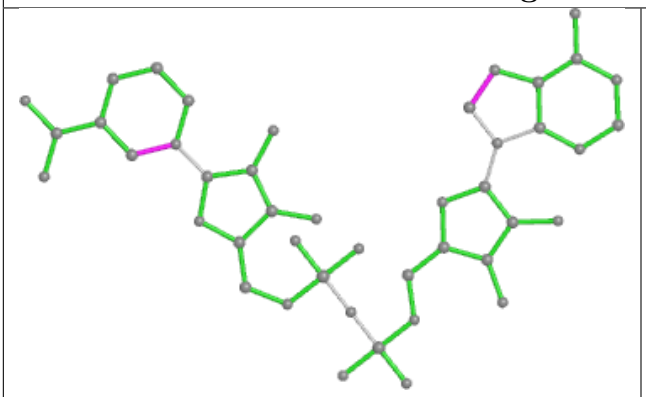


Torsions

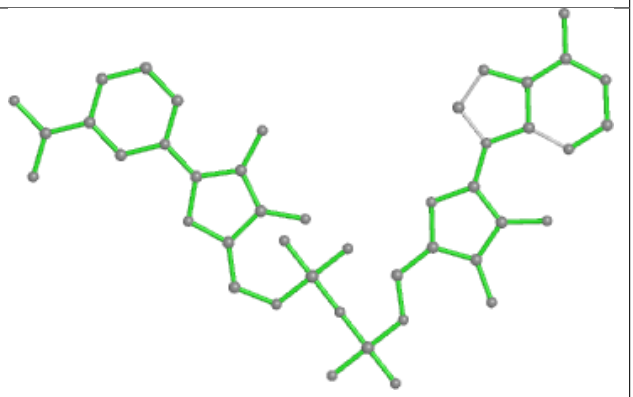


Rings

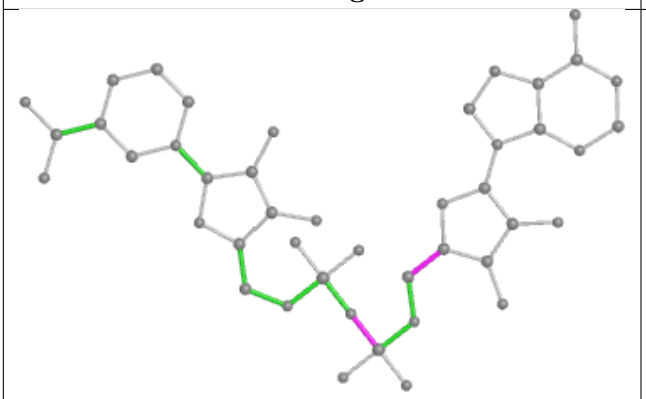
Ligand NAD B 401



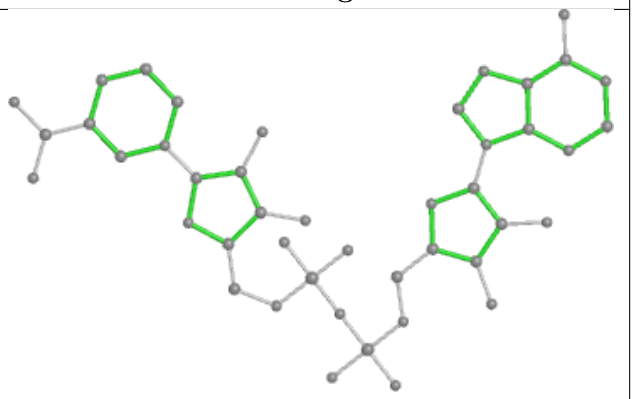
Bond lengths



Bond angles

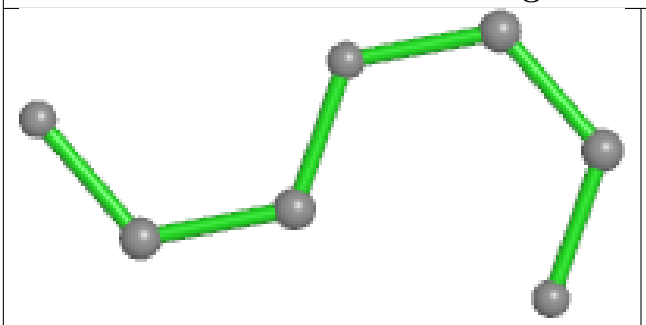


Torsions

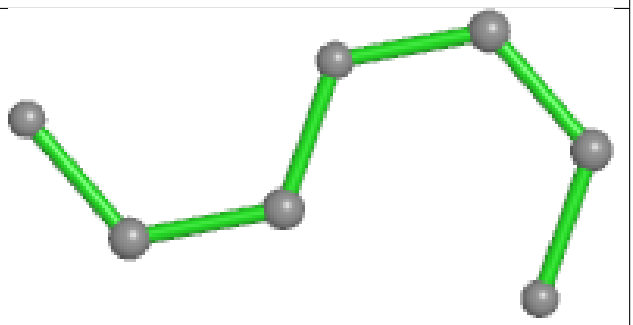


Rings

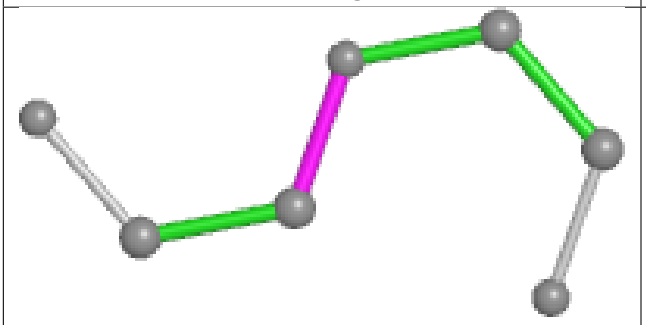
Ligand PEG D 402



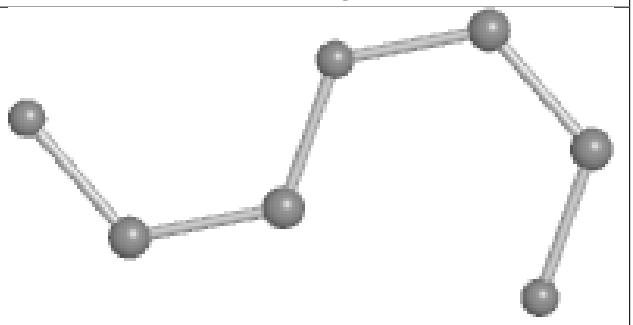
Bond lengths



Bond angles



Torsions



Rings

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	330/353 (93%)	-0.11	1 (0%) 94 93	29, 48, 79, 102	0
1	B	330/353 (93%)	-0.24	2 (0%) 89 88	27, 47, 79, 107	0
1	C	330/353 (93%)	0.88	53 (16%) 1 1	58, 92, 136, 179	0
1	D	320/353 (90%)	2.26	141 (44%) 0 0	70, 113, 154, 177	0
2	a	7/243 (2%)	0.42	0 100 100	64, 71, 92, 93	0
2	b	7/243 (2%)	0.01	0 100 100	70, 74, 98, 101	0
2	c	7/243 (2%)	1.30	2 (28%) 0 0	96, 106, 110, 110	0
All	All	1331/2141 (62%)	0.68	199 (14%) 2 1	27, 74, 139, 179	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	79	ALA	12.0
1	D	78	GLY	11.8
1	D	100	VAL	10.6
1	D	285	LEU	10.5
1	D	236	SER	10.2
1	D	65	THR	10.0
1	C	58	ALA	9.5
1	D	64	SER	9.4
1	D	273	GLY	9.3
1	D	85	ILE	9.0
1	C	155	ALA	8.7
1	D	313	ALA	8.4
1	D	34	PRO	8.3
1	D	68	ILE	7.7
1	D	75	GLU	7.6
1	D	35	LEU	7.5
1	D	162	VAL	7.5

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Mol	Chain	Res	Type	RSRZ
1	D	281	LEU	7.5
1	D	38	LEU	7.3
1	D	46	VAL	6.8
1	C	57	VAL	6.6
1	D	50	ILE	6.5
1	D	102	VAL	6.4
1	D	97	ALA	6.1
1	D	54	LEU	5.9
1	C	306	ALA	5.8
1	D	56	THR	5.7
1	D	37	ALA	5.7
1	D	104	ILE	5.7
1	C	168	ILE	5.5
1	D	74	ASN	5.4
1	C	162	VAL	5.4
1	C	281	LEU	5.4
1	D	254	ASN	5.4
1	D	344	ALA	5.1
1	D	142	ILE	5.1
1	D	77	VAL	5.0
1	D	189	GLY	5.0
1	D	87	LEU	4.9
1	D	111	VAL	4.9
1	D	310	LEU	4.8
1	D	196	ALA	4.7
1	D	121	ILE	4.7
1	D	41	GLY	4.6
1	D	53	ASP	4.6
1	D	52	LYS	4.5
1	D	51	LEU	4.4
1	C	285	LEU	4.4
1	D	33	ARG	4.4
1	C	95	PHE	4.4
1	C	142	ILE	4.4
1	C	303	PHE	4.4
1	D	42	ARG	4.3
1	D	101	ILE	4.3
1	C	278	GLU	4.3
1	C	265	ALA	4.3
1	D	333	MET	4.3
1	D	257	THR	4.3
1	D	264	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
2	c	318	ASP	4.2
1	D	290	ILE	4.2
1	D	180	GLY	4.2
1	D	352	SER	4.1
1	D	47	GLU	4.1
1	D	76	ALA	4.1
1	D	36	VAL	4.0
1	C	163	GLN	4.0
1	C	315	ASN	3.9
1	D	331	LEU	3.9
1	D	63	GLN	3.9
1	D	231	ASP	3.8
1	D	258	ILE	3.8
1	D	106	SER	3.8
1	D	192	GLY	3.8
1	D	71	LYS	3.8
1	D	66	GLN	3.8
1	D	174	GLY	3.7
1	C	75	GLU	3.7
1	C	308	GLY	3.7
1	D	57	VAL	3.7
1	D	343	ARG	3.6
1	D	283	GLN	3.6
1	D	91	ASP	3.6
1	D	284	ALA	3.6
1	D	223	VAL	3.6
1	C	68	ILE	3.5
1	C	293	ALA	3.5
1	C	164	SER	3.5
1	D	67	GLU	3.5
1	D	109	ASP	3.5
1	D	328	GLN	3.5
1	C	159	GLY	3.4
1	D	139	ILE	3.4
1	D	311	LYS	3.4
1	D	314	PRO	3.4
1	C	146	TYR	3.4
1	D	60	CYS	3.4
1	D	188	PHE	3.4
1	D	350	PRO	3.4
1	D	187	GLY	3.4
1	D	358	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	135	ALA	3.3
1	D	146	TYR	3.3
1	C	294	ALA	3.2
1	C	38	LEU	3.2
1	D	193	GLN	3.2
1	D	110	ASN	3.2
1	C	161	ARG	3.2
1	C	160	THR	3.2
1	C	325	TYR	3.2
1	C	300	SER	3.2
1	D	348	ARG	3.2
1	D	252	LEU	3.1
1	D	360	GLU	3.1
1	D	299	GLU	3.1
1	D	234	TYR	3.1
1	D	359	LYS	3.1
1	D	145	LEU	3.1
1	C	35	LEU	3.1
1	D	108	TYR	3.0
1	D	248	HIS	3.0
1	D	232	LEU	3.0
1	D	55	ALA	2.9
1	D	324	TRP	2.9
1	C	268	VAL	2.9
1	D	362	PHE	2.9
1	D	82	TYR	2.9
1	D	69	HIS	2.8
1	C	301	GLU	2.8
1	D	96	LYS	2.8
1	C	202	PHE	2.8
1	D	276	VAL	2.8
1	D	131	VAL	2.7
1	D	197	VAL	2.7
1	D	90	GLU	2.7
1	D	195	VAL	2.7
1	D	59	PHE	2.7
1	D	95	PHE	2.7
1	C	63	GLN	2.7
1	D	317	ILE	2.7
1	D	45	THR	2.7
1	D	138	THR	2.7
1	C	143	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	166	GLU	2.5
1	C	37	ALA	2.5
1	D	190	ARG	2.5
1	D	308	GLY	2.5
1	D	130	ALA	2.5
1	D	143	LEU	2.5
1	D	165	VAL	2.5
1	C	96	LYS	2.5
1	D	44	CYS	2.5
1	C	40	ASP	2.5
1	D	126	ILE	2.4
1	D	123	VAL	2.4
1	D	287	GLU	2.4
1	C	199	ALA	2.4
1	D	116	ALA	2.4
1	C	172	ALA	2.4
1	D	194	ALA	2.4
1	D	301	GLU	2.4
1	D	289	ARG	2.4
1	D	245	LEU	2.3
1	B	74	ASN	2.3
1	D	226	VAL	2.3
1	C	170	GLU	2.3
1	A	196	ALA	2.3
1	D	318	CYS	2.3
1	D	253	ILE	2.3
1	C	182	THR	2.3
1	D	134	THR	2.3
1	D	288	GLY	2.3
1	D	345	ILE	2.2
1	C	304	SER	2.2
1	C	39	LEU	2.2
1	D	242	HIS	2.2
1	D	302	PRO	2.2
2	c	317	LEU	2.2
1	D	356	CYS	2.2
1	D	280	ALA	2.1
1	C	48	MET	2.1
1	C	42	ARG	2.1
1	D	129	ALA	2.1
1	C	78	GLY	2.1
1	C	165	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	335	GLU	2.1
1	C	66	GLN	2.1
1	C	318	CYS	2.1
1	C	151	TRP	2.1
1	B	73	LEU	2.1
1	D	160	THR	2.1
1	D	191	THR	2.1
1	D	153	TYR	2.0
1	D	224	GLN	2.0
1	C	145	LEU	2.0
1	C	345	ILE	2.0
1	D	209	TYR	2.0
1	D	73	LEU	2.0
1	D	72	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

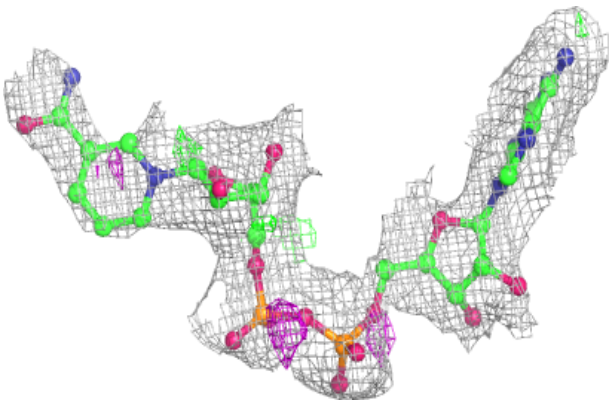
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

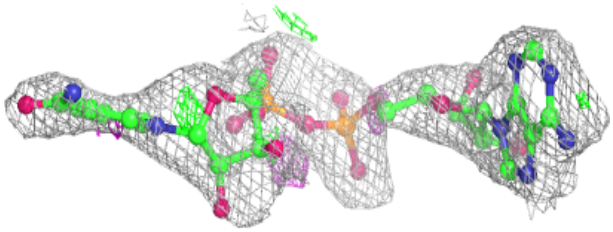
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAD	D	401	44/44	0.82	0.20	82,99,113,115	0
4	PEG	D	402	7/7	0.84	0.13	74,75,76,76	0
3	NAD	C	401	44/44	0.97	0.15	50,55,97,105	0
3	NAD	A	401	44/44	0.98	0.17	29,35,44,46	0
3	NAD	B	401	44/44	0.99	0.15	29,37,51,63	0

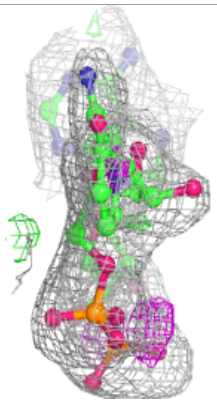
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

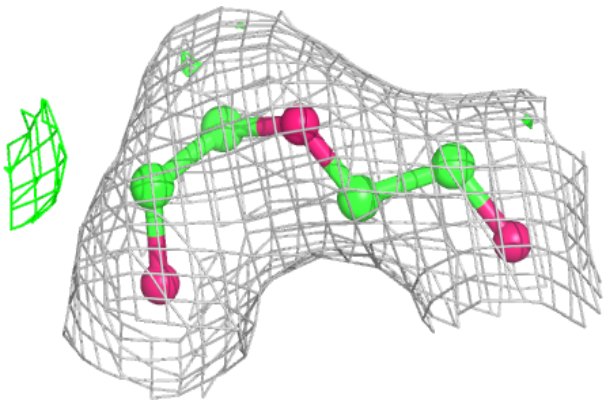


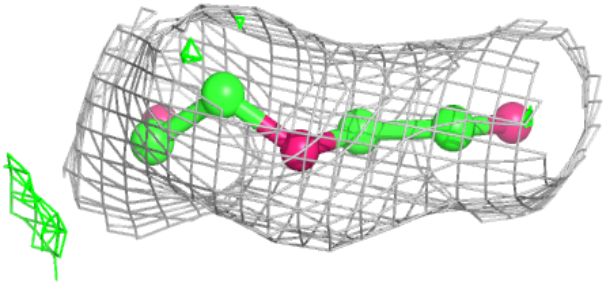


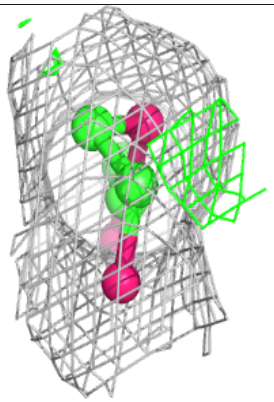


Electron density around PEG D 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

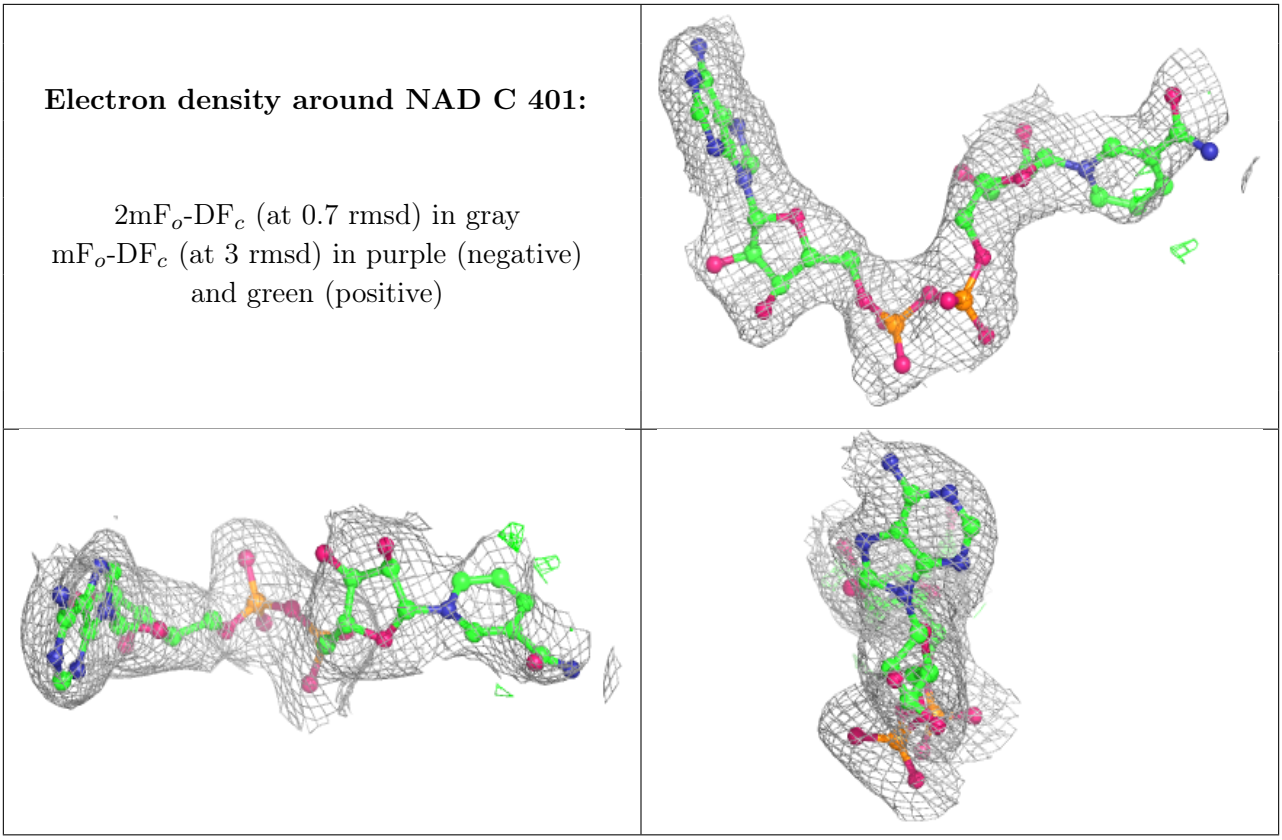






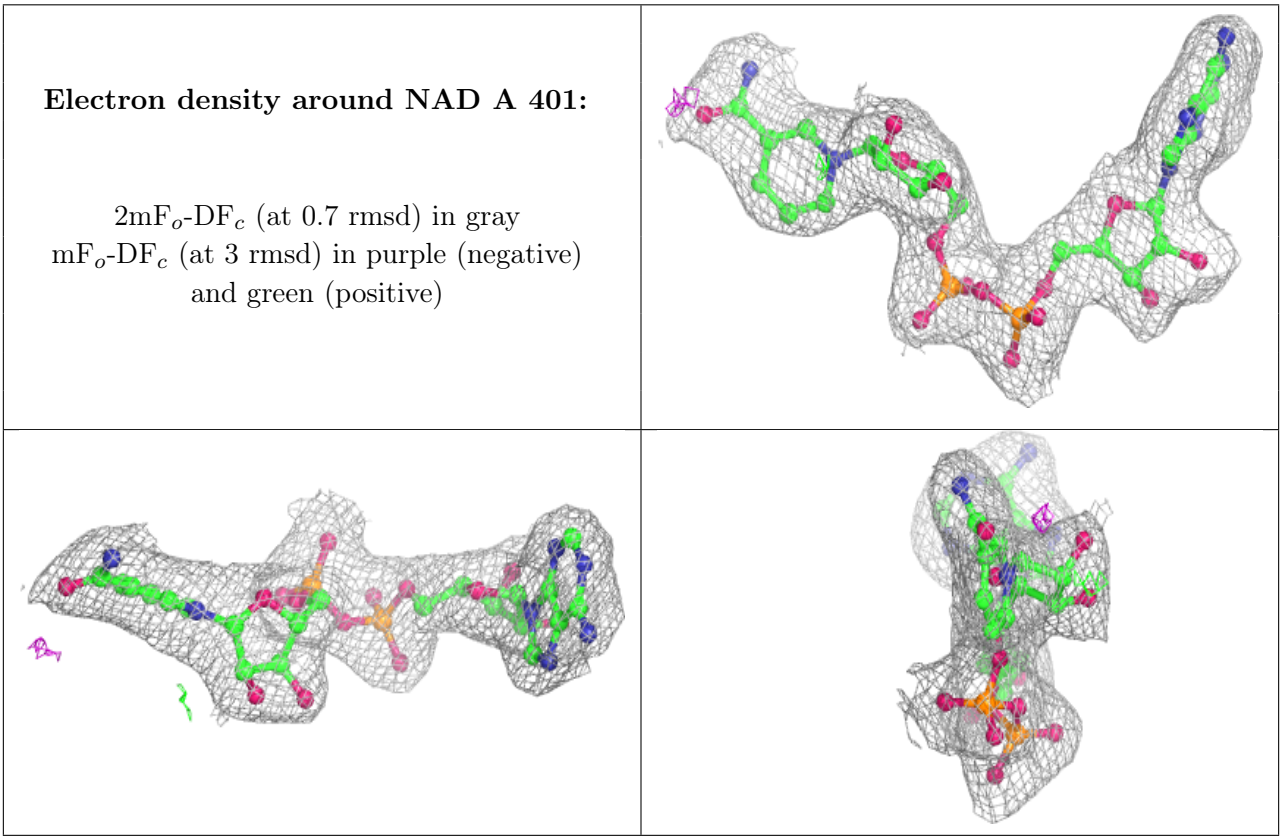
Electron density around NAD C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



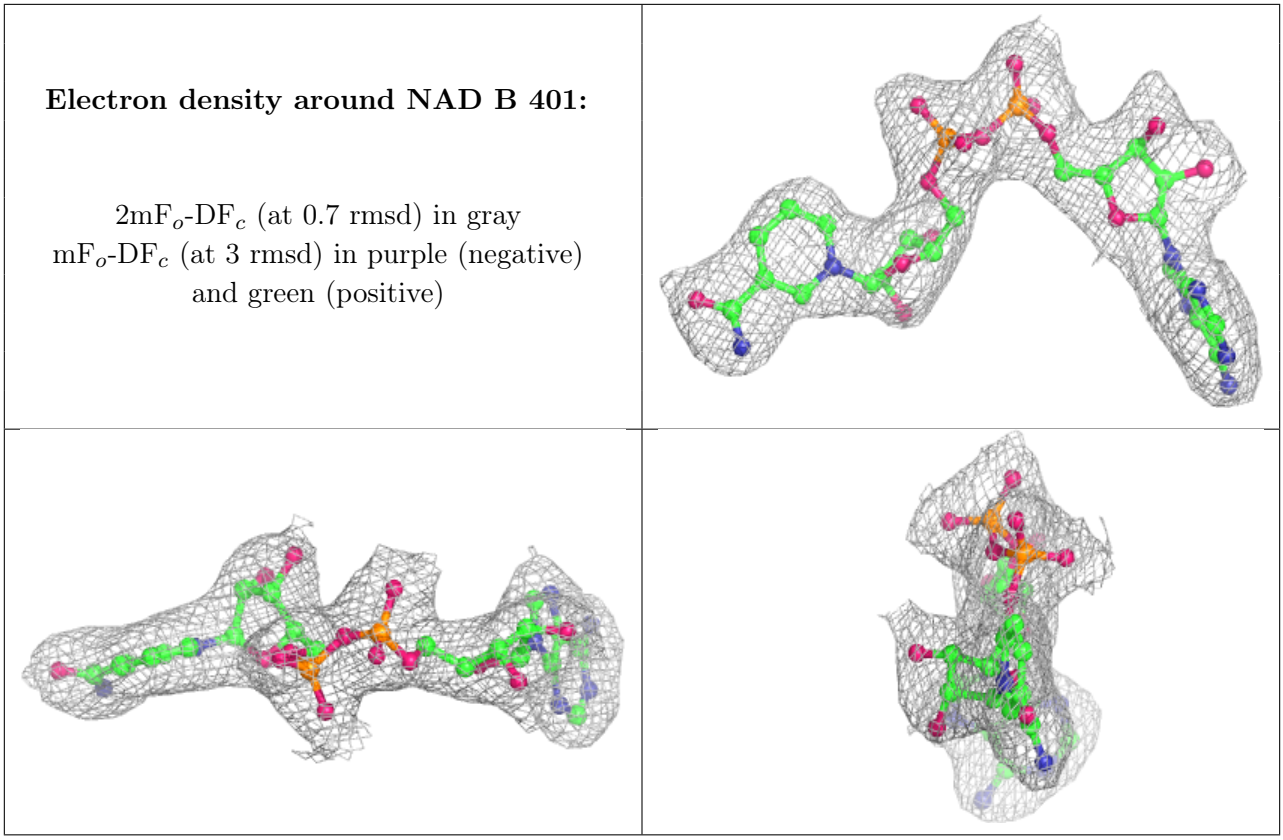
Electron density around NAD A 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAD B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.