



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 02:26 PM JST

PDB ID : 8ZN9 / pdb_00008zn9
Title : A vast marine sulfonate-based carbon cycle fueled by novel sulfoquinovosidases
Authors : Tang, K.; Ma, X.
Deposited on : 2024-05-26
Resolution : 1.80 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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

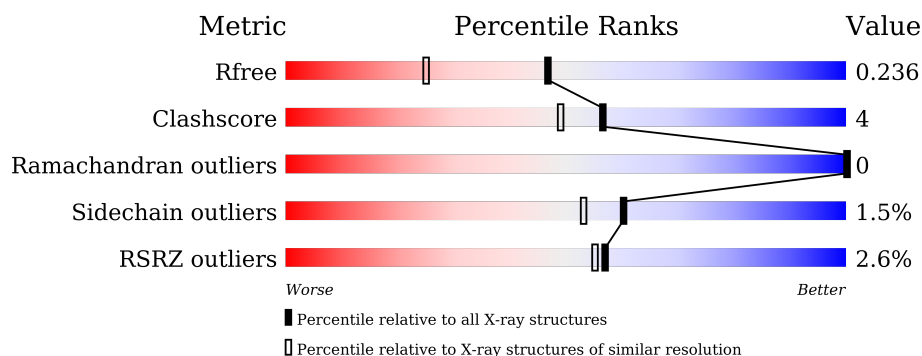
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 $\leq 5\%$. 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	400	<div> <div>3%</div> <div>86%7%6%</div> </div>
1	B	400	<div> <div>4%</div> <div>88%5%6%</div> </div>
1	C	400	<div> <div>2%</div> <div>79%11%9%</div> </div>
1	D	400	<div> <div>2%</div> <div>80%10%9%</div> </div>
1	E	400	<div> <div>0%</div> <div>84%6%10%</div> </div>
1	F	400	<div> <div>2%</div> <div>83%7%10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	C	1003	-	-	X	-
3	PEG	C	1004	-	-	X	-
3	PEG	C	1009	-	-	X	-
3	PEG	E	409	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19937 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 Oxidoreductase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	3	0
			2910	1845	516	530	19			
1	B	376	Total	C	N	O	S	0	4	0
			2915	1849	519	528	19			
1	C	363	Total	C	N	O	S	0	4	0
			2817	1793	494	510	20			
1	D	363	Total	C	N	O	S	0	4	0
			2817	1793	494	510	20			
1	E	362	Total	C	N	O	S	0	2	0
			2792	1777	490	506	19			
1	F	362	Total	C	N	O	S	0	3	0
			2799	1781	491	508	19			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q167F5
A	-34	GLY	-	expression tag	UNP Q167F5
A	-33	SER	-	expression tag	UNP Q167F5
A	-32	SER	-	expression tag	UNP Q167F5
A	-31	HIS	-	expression tag	UNP Q167F5
A	-30	HIS	-	expression tag	UNP Q167F5
A	-29	HIS	-	expression tag	UNP Q167F5
A	-28	HIS	-	expression tag	UNP Q167F5
A	-27	HIS	-	expression tag	UNP Q167F5
A	-26	HIS	-	expression tag	UNP Q167F5
A	-25	SER	-	expression tag	UNP Q167F5
A	-24	SER	-	expression tag	UNP Q167F5
A	-23	GLY	-	expression tag	UNP Q167F5
A	-22	LEU	-	expression tag	UNP Q167F5
A	-21	VAL	-	expression tag	UNP Q167F5
A	-19	PRO	-	expression tag	UNP Q167F5
A	-18	ARG	-	expression tag	UNP Q167F5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP Q167F5
A	-16	SER	-	expression tag	UNP Q167F5
A	-15	HIS	-	expression tag	UNP Q167F5
A	-14	MET	-	expression tag	UNP Q167F5
A	-13	ALA	-	expression tag	UNP Q167F5
A	-12	SER	-	expression tag	UNP Q167F5
A	-11	MET	-	expression tag	UNP Q167F5
A	-10	THR	-	expression tag	UNP Q167F5
A	-9	GLY	-	expression tag	UNP Q167F5
A	-8	GLY	-	expression tag	UNP Q167F5
A	-7	GLN	-	expression tag	UNP Q167F5
A	-6	GLN	-	expression tag	UNP Q167F5
A	-5	MET	-	expression tag	UNP Q167F5
A	-4	GLY	-	expression tag	UNP Q167F5
A	-3	ARG	-	expression tag	UNP Q167F5
A	-2	GLY	-	expression tag	UNP Q167F5
A	-1	SER	-	expression tag	UNP Q167F5
B	-35	MET	-	initiating methionine	UNP Q167F5
B	-34	GLY	-	expression tag	UNP Q167F5
B	-33	SER	-	expression tag	UNP Q167F5
B	-32	SER	-	expression tag	UNP Q167F5
B	-31	HIS	-	expression tag	UNP Q167F5
B	-30	HIS	-	expression tag	UNP Q167F5
B	-29	HIS	-	expression tag	UNP Q167F5
B	-28	HIS	-	expression tag	UNP Q167F5
B	-27	HIS	-	expression tag	UNP Q167F5
B	-26	HIS	-	expression tag	UNP Q167F5
B	-25	SER	-	expression tag	UNP Q167F5
B	-24	SER	-	expression tag	UNP Q167F5
B	-23	GLY	-	expression tag	UNP Q167F5
B	-22	LEU	-	expression tag	UNP Q167F5
B	-21	VAL	-	expression tag	UNP Q167F5
B	-19	PRO	-	expression tag	UNP Q167F5
B	-18	ARG	-	expression tag	UNP Q167F5
B	-17	GLY	-	expression tag	UNP Q167F5
B	-16	SER	-	expression tag	UNP Q167F5
B	-15	HIS	-	expression tag	UNP Q167F5
B	-14	MET	-	expression tag	UNP Q167F5
B	-13	ALA	-	expression tag	UNP Q167F5
B	-12	SER	-	expression tag	UNP Q167F5
B	-11	MET	-	expression tag	UNP Q167F5
B	-10	THR	-	expression tag	UNP Q167F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLY	-	expression tag	UNP Q167F5
B	-8	GLY	-	expression tag	UNP Q167F5
B	-7	GLN	-	expression tag	UNP Q167F5
B	-6	GLN	-	expression tag	UNP Q167F5
B	-5	MET	-	expression tag	UNP Q167F5
B	-4	GLY	-	expression tag	UNP Q167F5
B	-3	ARG	-	expression tag	UNP Q167F5
B	-2	GLY	-	expression tag	UNP Q167F5
B	-1	SER	-	expression tag	UNP Q167F5
C	-34	MET	-	initiating methionine	UNP Q167F5
C	-33	GLY	-	expression tag	UNP Q167F5
C	-32	SER	-	expression tag	UNP Q167F5
C	-31	SER	-	expression tag	UNP Q167F5
C	-30	HIS	-	expression tag	UNP Q167F5
C	-29	HIS	-	expression tag	UNP Q167F5
C	-28	HIS	-	expression tag	UNP Q167F5
C	-27	HIS	-	expression tag	UNP Q167F5
C	-26	HIS	-	expression tag	UNP Q167F5
C	-25	HIS	-	expression tag	UNP Q167F5
C	-24	SER	-	expression tag	UNP Q167F5
C	-23	SER	-	expression tag	UNP Q167F5
C	-22	GLY	-	expression tag	UNP Q167F5
C	-21	LEU	-	expression tag	UNP Q167F5
C	-20	VAL	-	expression tag	UNP Q167F5
C	-19	PRO	-	expression tag	UNP Q167F5
C	-18	ARG	-	expression tag	UNP Q167F5
C	-17	GLY	-	expression tag	UNP Q167F5
C	-16	SER	-	expression tag	UNP Q167F5
C	-15	HIS	-	expression tag	UNP Q167F5
C	-14	MET	-	expression tag	UNP Q167F5
C	-13	ALA	-	expression tag	UNP Q167F5
C	-12	SER	-	expression tag	UNP Q167F5
C	-11	MET	-	expression tag	UNP Q167F5
C	-10	THR	-	expression tag	UNP Q167F5
C	-9	GLY	-	expression tag	UNP Q167F5
C	-8	GLY	-	expression tag	UNP Q167F5
C	-7	GLN	-	expression tag	UNP Q167F5
C	-6	GLN	-	expression tag	UNP Q167F5
C	-5	MET	-	expression tag	UNP Q167F5
C	-4	GLY	-	expression tag	UNP Q167F5
C	-3	ARG	-	expression tag	UNP Q167F5
C	-2	GLY	-	expression tag	UNP Q167F5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q167F5
D	-34	MET	-	initiating methionine	UNP Q167F5
D	-33	GLY	-	expression tag	UNP Q167F5
D	-32	SER	-	expression tag	UNP Q167F5
D	-31	SER	-	expression tag	UNP Q167F5
D	-30	HIS	-	expression tag	UNP Q167F5
D	-29	HIS	-	expression tag	UNP Q167F5
D	-28	HIS	-	expression tag	UNP Q167F5
D	-27	HIS	-	expression tag	UNP Q167F5
D	-26	HIS	-	expression tag	UNP Q167F5
D	-25	HIS	-	expression tag	UNP Q167F5
D	-24	SER	-	expression tag	UNP Q167F5
D	-23	SER	-	expression tag	UNP Q167F5
D	-22	GLY	-	expression tag	UNP Q167F5
D	-21	LEU	-	expression tag	UNP Q167F5
D	-20	VAL	-	expression tag	UNP Q167F5
D	-19	PRO	-	expression tag	UNP Q167F5
D	-18	ARG	-	expression tag	UNP Q167F5
D	-17	GLY	-	expression tag	UNP Q167F5
D	-16	SER	-	expression tag	UNP Q167F5
D	-15	HIS	-	expression tag	UNP Q167F5
D	-14	MET	-	expression tag	UNP Q167F5
D	-13	ALA	-	expression tag	UNP Q167F5
D	-12	SER	-	expression tag	UNP Q167F5
D	-11	MET	-	expression tag	UNP Q167F5
D	-10	THR	-	expression tag	UNP Q167F5
D	-9	GLY	-	expression tag	UNP Q167F5
D	-8	GLY	-	expression tag	UNP Q167F5
D	-7	GLN	-	expression tag	UNP Q167F5
D	-6	GLN	-	expression tag	UNP Q167F5
D	-5	MET	-	expression tag	UNP Q167F5
D	-4	GLY	-	expression tag	UNP Q167F5
D	-3	ARG	-	expression tag	UNP Q167F5
D	-2	GLY	-	expression tag	UNP Q167F5
D	-1	SER	-	expression tag	UNP Q167F5
E	-34	MET	-	initiating methionine	UNP Q167F5
E	-33	GLY	-	expression tag	UNP Q167F5
E	-32	SER	-	expression tag	UNP Q167F5
E	-31	SER	-	expression tag	UNP Q167F5
E	-30	HIS	-	expression tag	UNP Q167F5
E	-29	HIS	-	expression tag	UNP Q167F5
E	-28	HIS	-	expression tag	UNP Q167F5

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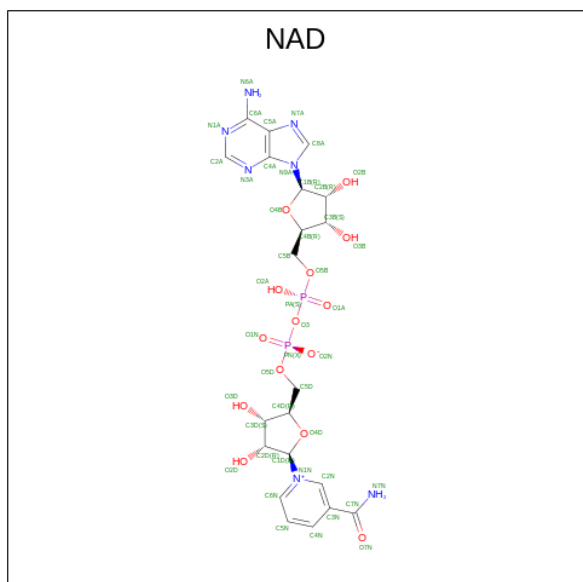
Chain	Residue	Modelled	Actual	Comment	Reference
E	-27	HIS	-	expression tag	UNP Q167F5
E	-26	HIS	-	expression tag	UNP Q167F5
E	-25	HIS	-	expression tag	UNP Q167F5
E	-24	SER	-	expression tag	UNP Q167F5
E	-23	SER	-	expression tag	UNP Q167F5
E	-22	GLY	-	expression tag	UNP Q167F5
E	-21	LEU	-	expression tag	UNP Q167F5
E	-20	VAL	-	expression tag	UNP Q167F5
E	-19	PRO	-	expression tag	UNP Q167F5
E	-18	ARG	-	expression tag	UNP Q167F5
E	-17	GLY	-	expression tag	UNP Q167F5
E	-16	SER	-	expression tag	UNP Q167F5
E	-15	HIS	-	expression tag	UNP Q167F5
E	-14	MET	-	expression tag	UNP Q167F5
E	-13	ALA	-	expression tag	UNP Q167F5
E	-12	SER	-	expression tag	UNP Q167F5
E	-11	MET	-	expression tag	UNP Q167F5
E	-10	THR	-	expression tag	UNP Q167F5
E	-9	GLY	-	expression tag	UNP Q167F5
E	-8	GLY	-	expression tag	UNP Q167F5
E	-7	GLN	-	expression tag	UNP Q167F5
E	-6	GLN	-	expression tag	UNP Q167F5
E	-5	MET	-	expression tag	UNP Q167F5
E	-4	GLY	-	expression tag	UNP Q167F5
E	-3	ARG	-	expression tag	UNP Q167F5
E	-2	GLY	-	expression tag	UNP Q167F5
E	-1	SER	-	expression tag	UNP Q167F5
F	-34	MET	-	initiating methionine	UNP Q167F5
F	-33	GLY	-	expression tag	UNP Q167F5
F	-32	SER	-	expression tag	UNP Q167F5
F	-31	SER	-	expression tag	UNP Q167F5
F	-30	HIS	-	expression tag	UNP Q167F5
F	-29	HIS	-	expression tag	UNP Q167F5
F	-28	HIS	-	expression tag	UNP Q167F5
F	-27	HIS	-	expression tag	UNP Q167F5
F	-26	HIS	-	expression tag	UNP Q167F5
F	-25	HIS	-	expression tag	UNP Q167F5
F	-24	SER	-	expression tag	UNP Q167F5
F	-23	SER	-	expression tag	UNP Q167F5
F	-22	GLY	-	expression tag	UNP Q167F5
F	-21	LEU	-	expression tag	UNP Q167F5
F	-20	VAL	-	expression tag	UNP Q167F5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	PRO	-	expression tag	UNP Q167F5
F	-18	ARG	-	expression tag	UNP Q167F5
F	-17	GLY	-	expression tag	UNP Q167F5
F	-16	SER	-	expression tag	UNP Q167F5
F	-15	HIS	-	expression tag	UNP Q167F5
F	-14	MET	-	expression tag	UNP Q167F5
F	-13	ALA	-	expression tag	UNP Q167F5
F	-12	SER	-	expression tag	UNP Q167F5
F	-11	MET	-	expression tag	UNP Q167F5
F	-10	THR	-	expression tag	UNP Q167F5
F	-9	GLY	-	expression tag	UNP Q167F5
F	-8	GLY	-	expression tag	UNP Q167F5
F	-7	GLN	-	expression tag	UNP Q167F5
F	-6	GLN	-	expression tag	UNP Q167F5
F	-5	MET	-	expression tag	UNP Q167F5
F	-4	GLY	-	expression tag	UNP Q167F5
F	-3	ARG	-	expression tag	UNP Q167F5
F	-2	GLY	-	expression tag	UNP Q167F5
F	-1	SER	-	expression tag	UNP Q167F5

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



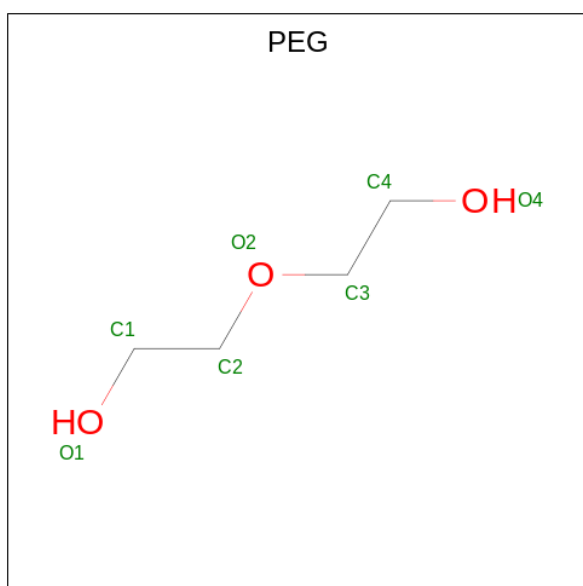
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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

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

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

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

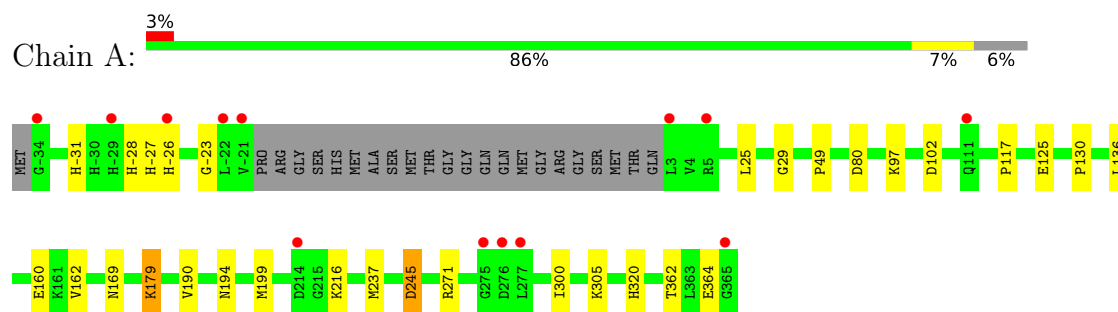
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	382	Total	O	0	0
			382	382		
4	B	374	Total	O	0	0
			374	374		
4	C	330	Total	O	0	0
			330	330		
4	D	328	Total	O	0	0
			328	328		
4	E	356	Total	O	0	0
			356	356		
4	F	356	Total	O	0	0
			356	356		

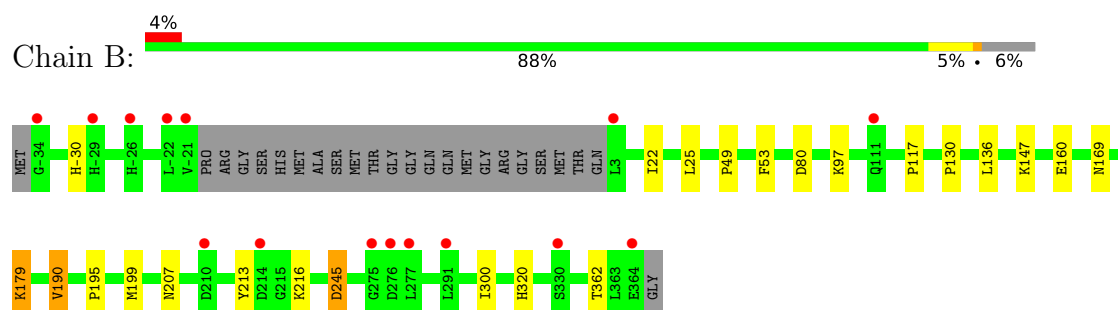
3 Residue-property plots [i](#)

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.

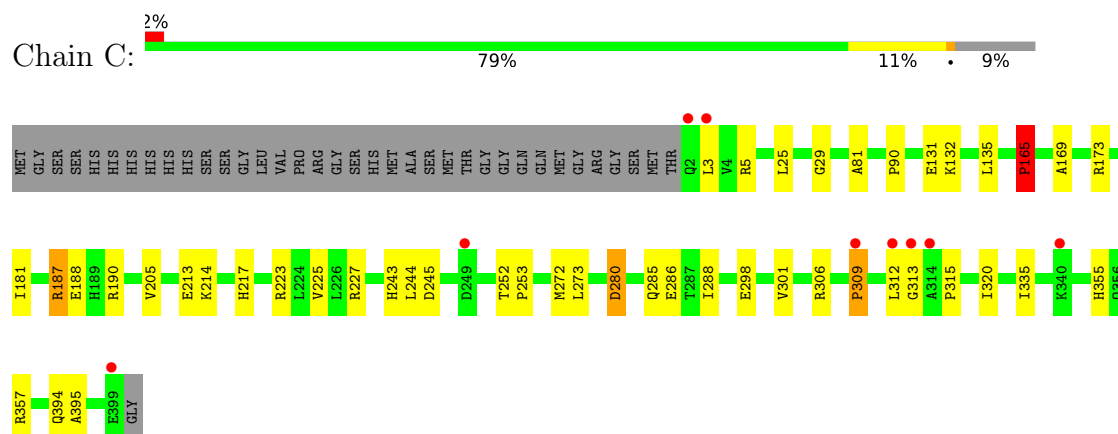
- Molecule 1: Oxidoreductase, putative



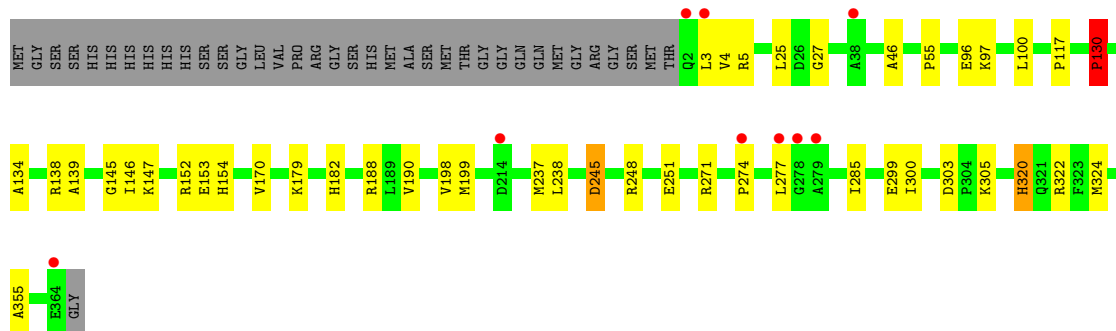
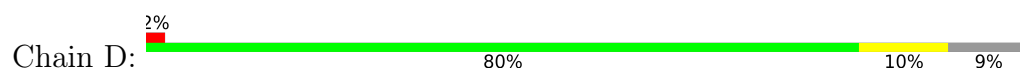
- Molecule 1: Oxidoreductase, putative



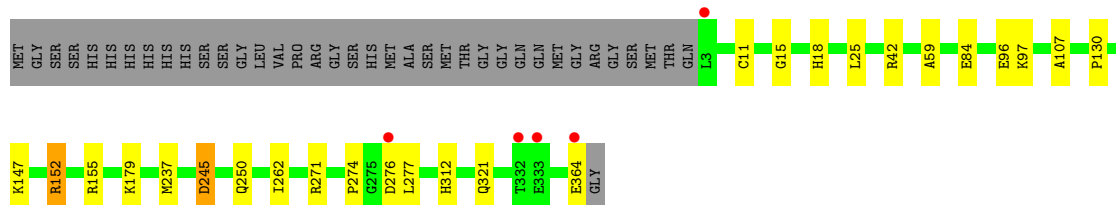
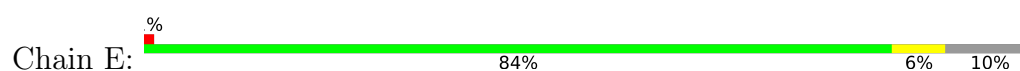
- Molecule 1: Oxidoreductase, putative



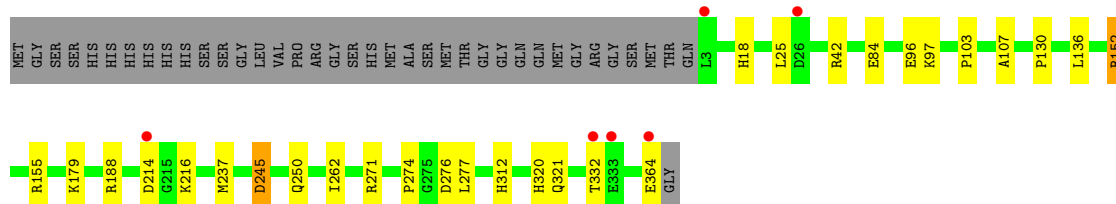
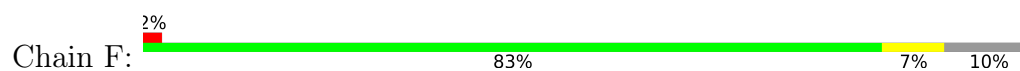
- Molecule 1: Oxidoreductase, putative



- Molecule 1: Oxidoreductase, putative



- Molecule 1: Oxidoreductase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.92Å 56.69Å 217.30Å 90.00° 96.10° 90.00°	Depositor
Resolution (Å)	30.48 – 1.80 30.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.48-1.80) 99.4 (30.48-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.67Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.238 0.218 , 0.236	Depositor DCC
R_{free} test set	14453 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19937	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7411e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.19	2/2982 (0.1%)	1.20	4/4052 (0.1%)
1	B	1.16	5/2987 (0.2%)	1.16	4/4060 (0.1%)
1	C	1.22	7/2884 (0.2%)	1.22	4/3922 (0.1%)
1	D	1.22	6/2884 (0.2%)	1.22	3/3922 (0.1%)
1	E	1.18	5/2859 (0.2%)	1.23	3/3888 (0.1%)
1	F	1.20	7/2866 (0.2%)	1.25	3/3898 (0.1%)
All	All	1.20	32/17462 (0.2%)	1.21	21/23742 (0.1%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	HIS	CE1-NE2	7.82	1.40	1.32
1	D	182	HIS	CE1-NE2	7.08	1.39	1.32
1	B	117	PRO	C-O	-6.98	1.16	1.23
1	A	117	PRO	C-O	-6.87	1.16	1.23
1	E	84	GLU	C-O	6.17	1.31	1.24
1	E	18	HIS	CE1-NE2	6.08	1.38	1.32
1	C	309	PRO	C-O	6.00	1.30	1.23
1	D	238	LEU	C-O	5.87	1.31	1.24
1	F	214	ASP	C-O	5.72	1.31	1.23
1	F	312	HIS	CE1-NE2	5.67	1.38	1.32
1	F	84	GLU	C-O	5.58	1.30	1.24
1	F	18	HIS	CE1-NE2	5.54	1.38	1.32
1	C	81	ALA	C-O	5.53	1.31	1.24
1	E	312	HIS	CE1-NE2	5.53	1.38	1.32
1	D	320	HIS	CE1-NE2	5.50	1.38	1.32
1	F	107	ALA	C-O	5.50	1.30	1.24
1	C	273	LEU	C-O	5.46	1.30	1.24
1	C	90	PRO	C-O	-5.43	1.17	1.24
1	B	22	ILE	C-O	5.39	1.30	1.24
1	B	190	VAL	C-O	5.33	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	PRO	C-O	-5.32	1.17	1.24
1	C	243	HIS	CE1-NE2	5.30	1.37	1.32
1	A	49	PRO	C-O	-5.26	1.17	1.24
1	C	313	GLY	C-O	5.24	1.32	1.23
1	E	262	ILE	C-O	5.22	1.29	1.24
1	F	262	ILE	C-O	5.20	1.29	1.24
1	D	139	ALA	C-O	-5.17	1.18	1.24
1	E	107	ALA	C-O	5.15	1.30	1.24
1	D	55	PRO	C-O	-5.14	1.17	1.24
1	F	136	LEU	C-O	5.11	1.30	1.24
1	B	195	PRO	C-O	-5.05	1.18	1.23
1	D	46	ALA	C-O	5.01	1.30	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	198	VAL	O-C-N	9.76	133.55	123.10
1	F	332	THR	CA-CB-OG1	-7.73	98.00	109.60
1	C	315	PRO	O-C-N	-7.38	117.91	121.31
1	C	280	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	80	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	130	PRO	N-CA-C	6.16	118.21	110.70
1	A	130	PRO	N-CA-C	5.91	117.91	110.70
1	D	245	ASP	CA-CB-CG	5.89	118.49	112.60
1	F	130	PRO	N-CA-C	5.80	117.78	110.70
1	B	80	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	130	PRO	N-CA-C	5.68	117.62	110.70
1	E	130	PRO	N-CA-C	5.63	117.57	110.70
1	A	102	ASP	CB-CA-C	5.53	116.15	109.85
1	B	245	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	165	PRO	N-CA-C	5.46	117.36	110.70
1	A	245	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	245	ASP	CA-CB-CG	5.22	117.82	112.60
1	C	213	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	207	ASN	N-CA-C	5.10	117.83	110.28
1	F	245	ASP	CA-CB-CG	5.06	117.66	112.60
1	E	276	ASP	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2910	0	2870	20	0
1	B	2915	0	2882	16	0
1	C	2817	0	2806	38	0
1	D	2817	0	2806	31	0
1	E	2792	0	2779	18	0
1	F	2799	0	2785	15	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
2	E	44	0	26	1	0
2	F	44	0	26	2	0
3	A	84	0	120	11	0
3	B	105	0	150	9	0
3	C	77	0	110	24	0
3	D	84	0	120	11	0
3	E	70	0	100	11	0
3	F	77	0	109	8	0
4	A	382	0	0	6	0
4	B	374	0	0	8	0
4	C	330	0	0	5	1
4	D	328	0	0	5	1
4	E	356	0	0	4	1
4	F	356	0	0	5	1
All	All	19937	0	17793	159	2

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 4.

All (159) 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:A:194:ASN:HD21	3:A:403:PEG:H22	1.32	0.95
1:C:187:ARG:HG2	1:C:187:ARG:HH11	1.29	0.94
1:B:-30:HIS:HD2	4:B:528:HOH:O	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:HD3	3:C:1003:PEG:H41	1.47	0.93
3:D:404:PEG:H41	4:D:667:HOH:O	1.69	0.93
1:D:274:PRO:HD2	1:D:277:LEU:HD12	1.58	0.84
1:B:160:GLU:O	3:B:411:PEG:H32	1.79	0.82
1:E:152:ARG:HH21	1:E:152:ARG:HG2	1.43	0.81
1:E:147:LYS:NZ	3:E:402:PEG:H32	1.96	0.80
1:F:152:ARG:HH21	1:F:152:ARG:HG2	1.46	0.80
1:C:173:ARG:HH21	3:C:1004:PEG:H21	1.51	0.75
1:D:305:LYS:HG3	3:D:408:PEG:H42	1.67	0.74
1:B:147:LYS:NZ	3:B:402:PEG:H22	2.03	0.73
1:D:152:ARG:HD3	1:D:154:HIS:CD2	2.24	0.72
3:D:404:PEG:C4	4:D:667:HOH:O	2.32	0.71
1:E:59:ALA:HB1	3:E:409:PEG:H12	1.73	0.69
1:A:169:ASN:HB3	3:A:411:PEG:H41	1.74	0.69
3:E:403:PEG:H32	4:E:770:HOH:O	1.93	0.69
4:B:744:HOH:O	3:E:409:PEG:H31	1.93	0.69
3:C:1009:PEG:H32	4:C:1298:HOH:O	1.92	0.69
1:A:216:LYS:NZ	4:A:501:HOH:O	2.18	0.68
1:C:309:PRO:HD2	1:C:312:LEU:HD12	1.75	0.68
1:B:-30:HIS:CD2	4:B:528:HOH:O	2.34	0.68
1:C:173:ARG:HH21	3:C:1004:PEG:C2	2.07	0.67
3:E:406:PEG:H21	4:E:692:HOH:O	1.95	0.67
1:A:160:GLU:O	3:A:408:PEG:H31	1.96	0.66
1:B:147:LYS:HZ3	3:B:402:PEG:H22	1.60	0.66
1:A:-31:HIS:HE1	1:A:364:GLU:OE1	1.78	0.66
3:C:1009:PEG:C3	4:C:1298:HOH:O	2.44	0.66
1:E:147:LYS:HZ2	3:E:402:PEG:H32	1.59	0.66
1:D:147:LYS:HE2	3:D:402:PEG:H31	1.78	0.65
1:B:216:LYS:HG2	4:B:843:HOH:O	1.96	0.65
1:D:145:GLY:HA3	3:D:402:PEG:H32	1.77	0.65
3:F:403:PEG:H12	4:F:678:HOH:O	1.98	0.64
1:A:-31:HIS:HD2	1:A:-26:HIS:ND1	1.97	0.63
1:C:25:LEU:HD11	1:C:355:HIS:HB3	1.80	0.62
1:D:25:LEU:HD11	1:D:320:HIS:HB3	1.82	0.62
1:E:42:ARG:HD3	4:E:625:HOH:O	2.01	0.61
1:F:42:ARG:HD3	4:F:586:HOH:O	2.01	0.60
1:C:306:ARG:HD3	3:C:1012:PEG:H12	1.83	0.60
1:F:216:LYS:NZ	3:F:412:PEG:H41	2.17	0.59
1:A:194:ASN:ND2	3:A:403:PEG:H22	2.11	0.59
1:C:188:GLU:OE2	1:C:286:GLU:HG3	2.02	0.58
3:F:406:PEG:H11	4:F:762:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:CD	3:C:1003:PEG:H41	2.29	0.58
1:B:25:LEU:HD11	1:B:320:HIS:HB3	1.86	0.57
1:C:245:ASP:H	3:C:1009:PEG:C1	2.18	0.57
3:E:406:PEG:H22	4:E:516:HOH:O	2.03	0.57
1:A:25:LEU:HD11	1:A:320:HIS:HB3	1.86	0.57
1:F:188:ARG:O	3:F:407:PEG:H22	2.06	0.56
1:B:300:ILE:HG22	1:B:300:ILE:O	2.06	0.55
1:C:395:ALA:O	3:C:1010:PEG:H32	2.06	0.55
1:E:152:ARG:HG2	1:E:152:ARG:NH2	2.19	0.55
2:F:401:NAD:C6N	4:F:707:HOH:O	2.55	0.55
1:B:362[A]:THR:HG23	4:B:746:HOH:O	2.06	0.55
1:A:199:MET:HE2	4:A:700:HOH:O	2.06	0.54
1:D:130:PRO:HG3	3:D:407:PEG:H42	1.90	0.54
1:A:-23:GLY:CA	1:A:362:THR:HG21	2.38	0.53
3:C:1003:PEG:H31	4:C:1266:HOH:O	2.08	0.53
1:E:271:ARG:HD2	3:E:411:PEG:H32	1.89	0.53
1:F:103:PRO:HB3	3:F:406:PEG:H41	1.90	0.53
1:C:320:ILE:HG12	1:C:335[A]:ILE:HD11	1.90	0.53
1:D:285:ILE:HG12	1:D:300[A]:ILE:HD11	1.89	0.53
1:C:187:ARG:HH11	1:C:187:ARG:CG	2.12	0.53
1:C:187:ARG:HG2	1:C:187:ARG:NH1	2.07	0.52
1:F:271:ARG:O	3:F:410:PEG:H42	2.08	0.52
1:C:165:PRO:HG3	3:C:1011:PEG:H11	1.91	0.52
1:A:271:ARG:HD3	3:A:406:PEG:H22	1.91	0.52
1:F:274:PRO:HB2	1:F:276:ASP:OD1	2.10	0.52
1:D:153:GLU:OE1	1:D:251:GLU:HG3	2.11	0.51
1:E:147:LYS:HZ3	3:E:402:PEG:H32	1.74	0.51
1:F:152:ARG:HG2	1:F:152:ARG:NH2	2.21	0.50
1:C:205:VAL:HA	3:C:1005:PEG:H41	1.93	0.50
1:C:244:LEU:N	3:C:1009:PEG:H11	2.27	0.50
1:D:274:PRO:HD2	1:D:277:LEU:CD1	2.37	0.50
1:F:96:GLU:OE2	2:F:401:NAD:H2N	2.12	0.50
1:F:274:PRO:HG2	1:F:277:LEU:HG	1.94	0.50
1:D:248:ARG:NH1	4:D:505:HOH:O	2.45	0.50
1:B:199:MET:HE2	4:B:692:HOH:O	2.11	0.49
3:A:406:PEG:O1	4:A:502:HOH:O	2.20	0.49
1:E:274:PRO:HG2	1:E:277:LEU:CD1	2.42	0.49
1:C:306:ARG:HD3	3:C:1012:PEG:H31	1.94	0.49
1:C:29:GLY:HA3	3:C:1006:PEG:H32	1.95	0.49
1:F:216:LYS:HZ2	3:F:412:PEG:H41	1.76	0.49
1:E:59:ALA:HB2	3:E:409:PEG:H41	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:PRO:HG2	1:E:277:LEU:HG	1.96	0.48
1:B:136:LEU:HD23	1:B:190:VAL:HG22	1.96	0.48
1:D:188:ARG:NH2	3:D:404:PEG:H12	2.28	0.48
1:D:170:VAL:HG23	3:D:405:PEG:H21	1.96	0.48
1:E:59:ALA:HB1	3:E:409:PEG:C1	2.40	0.48
1:E:25:LEU:HD21	1:E:321:GLN:HG2	1.96	0.47
1:C:223:ARG:NH2	3:C:1003:PEG:H22	2.28	0.47
1:D:322[A]:ARG:NH2	4:D:502:HOH:O	2.27	0.47
1:C:394:GLN:HB2	3:C:1010:PEG:H21	1.97	0.47
3:F:403:PEG:H32	4:F:623:HOH:O	2.14	0.47
3:B:404:PEG:H21	4:B:809:HOH:O	2.16	0.46
1:B:53:PHE:HB2	3:B:408:PEG:H22	1.98	0.46
1:D:146:ILE:HD13	1:D:190:VAL:CG1	2.46	0.46
1:E:96:GLU:OE2	2:E:401:NAD:H2N	2.16	0.46
3:B:409:PEG:H22	3:B:409:PEG:H41	1.35	0.46
1:A:136:LEU:HD23	1:A:190:VAL:HG22	1.98	0.46
1:C:190:ARG:HB3	1:C:285:GLN:HG3	1.98	0.46
1:A:179:LYS:HA	1:A:179:LYS:HE2	1.96	0.46
1:F:25:LEU:HD21	1:F:321:GLN:HG2	1.98	0.46
1:C:181:ILE:HD13	1:C:225:VAL:CG1	2.46	0.45
1:D:117:PRO:HA	3:D:412:PEG:H32	1.97	0.45
1:C:173:ARG:NH2	3:C:1004:PEG:H42	2.31	0.45
1:E:237:MET:HE3	1:E:237:MET:HB3	1.80	0.45
1:C:272:MET:HE3	1:C:272:MET:HB3	1.76	0.45
1:A:29:GLY:HA3	3:A:404:PEG:H42	1.97	0.45
1:A:162:VAL:HG22	3:A:408:PEG:H12	1.98	0.45
1:A:237:MET:HE3	1:A:237:MET:HB3	1.75	0.45
1:D:96:GLU:OE2	2:D:401:NAD:H2N	2.17	0.45
1:B:-30:HIS:CG	1:B:213:TYR:CE2	3.05	0.44
3:C:1004:PEG:H21	3:C:1004:PEG:H42	1.77	0.44
3:A:410:PEG:H42	4:A:531:HOH:O	2.17	0.44
1:C:173:ARG:HG3	1:C:173:ARG:HH11	1.83	0.44
1:D:271:ARG:HD3	3:D:413:PEG:H22	1.99	0.44
1:D:138:ARG:HG3	1:D:138:ARG:HH11	1.81	0.43
3:C:1006:PEG:H31	4:C:1172:HOH:O	2.17	0.43
1:D:303:ASP:HA	3:D:411:PEG:H21	2.01	0.43
3:A:413:PEG:H32	3:A:413:PEG:H12	1.85	0.43
1:C:357[A]:ARG:NH2	4:C:1101:HOH:O	2.25	0.42
1:C:173:ARG:NH2	3:C:1004:PEG:H21	2.28	0.42
1:D:3:LEU:HD12	1:D:27:GLY:C	2.43	0.42
1:C:223:ARG:CZ	3:C:1003:PEG:H22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:413:PEG:H22	1:D:355:ALA:O	2.19	0.42
1:C:286:GLU:HB2	1:C:301:VAL:HB	2.02	0.42
1:D:4:VAL:HG21	1:D:324:MET:HG3	2.02	0.42
1:C:252:THR:O	1:C:253:PRO:C	2.63	0.42
1:F:155:ARG:HB3	1:F:250:GLN:HG3	2.01	0.42
1:C:135:LEU:C	1:C:135:LEU:HD12	2.45	0.41
1:D:3:LEU:HD23	1:D:5:ARG:CD	2.50	0.41
1:D:199[A]:MET:HE3	1:D:199[A]:MET:HB2	1.93	0.41
1:B:169:ASN:HB3	3:B:415:PEG:H31	2.02	0.41
1:B:179:LYS:HE2	1:B:179:LYS:HA	2.02	0.41
1:C:131:GLU:OE2	2:C:1001:NAD:H2N	2.19	0.41
1:C:244:LEU:H	3:C:1009:PEG:H11	1.85	0.41
1:C:288:ILE:O	1:C:298:GLU:HA	2.20	0.41
1:D:299:GLU:O	1:D:300[B]:ILE:HD13	2.21	0.41
1:F:237:MET:HB3	1:F:237:MET:HE3	1.82	0.41
1:D:237:MET:HE3	1:D:237:MET:HB3	1.74	0.41
1:E:25:LEU:HD23	1:E:25:LEU:HA	1.90	0.41
1:E:155:ARG:HB3	1:E:250:GLN:HG3	2.02	0.41
1:B:147:LYS:HZ2	3:B:402:PEG:H22	1.82	0.41
1:A:-27:HIS:CE1	4:A:707:HOH:O	2.74	0.40
1:C:3:LEU:HD23	1:C:5:ARG:CD	2.51	0.40
1:A:-31:HIS:CD2	1:A:-26:HIS:ND1	2.83	0.40
1:A:125:GLU:OE1	2:A:401:NAD:N7N	2.48	0.40
1:F:25:LEU:HD11	1:F:320:HIS:HB3	2.03	0.40
1:C:169:ALA:CB	1:C:335[A]:ILE:HD13	2.51	0.40
1:D:199[A]:MET:HE2	4:D:677:HOH:O	2.20	0.40
1:D:305:LYS:HE3	1:D:305:LYS:HB2	1.80	0.40
3:B:404:PEG:H41	4:B:615:HOH:O	2.21	0.40
1:D:100:LEU:C	1:D:100:LEU:HD12	2.46	0.40
1:E:11:CYS:HA	1:E:15:GLY:HA3	2.03	0.40
1:A:-28:HIS:HB2	4:A:510:HOH:O	2.20	0.40
1:C:205:VAL:HG23	3:C:1005:PEG:H11	2.03	0.40
1:D:134:ALA:CB	1:D:300[A]:ILE:HD13	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1297:HOH:O	4:F:773:HOH:O[1_565]	2.13	0.07
4:D:689:HOH:O	4:E:775:HOH:O[1_565]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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	376/400 (94%)	371 (99%)	5 (1%)	0	100	100
1	B	376/400 (94%)	372 (99%)	4 (1%)	0	100	100
1	C	365/400 (91%)	360 (99%)	5 (1%)	0	100	100
1	D	365/400 (91%)	359 (98%)	6 (2%)	0	100	100
1	E	362/400 (90%)	358 (99%)	4 (1%)	0	100	100
1	F	363/400 (91%)	359 (99%)	4 (1%)	0	100	100
All	All	2207/2400 (92%)	2179 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	302/316 (96%)	297 (98%)	5 (2%)	56	47
1	B	303/316 (96%)	300 (99%)	3 (1%)	73	68
1	C	292/316 (92%)	287 (98%)	5 (2%)	56	47
1	D	292/316 (92%)	288 (99%)	4 (1%)	62	56
1	E	289/316 (92%)	284 (98%)	5 (2%)	56	47
1	F	290/316 (92%)	285 (98%)	5 (2%)	56	47
All	All	1768/1896 (93%)	1741 (98%)	27 (2%)	60	53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	179	LYS
1	A	245	ASP
1	A	300	ILE
1	A	305	LYS
1	B	97	LYS
1	B	179	LYS
1	B	245	ASP
1	C	132	LYS
1	C	165	PRO
1	C	187	ARG
1	C	214	LYS
1	C	280	ASP
1	D	97	LYS
1	D	130	PRO
1	D	179	LYS
1	D	245	ASP
1	E	97	LYS
1	E	152	ARG
1	E	179	LYS
1	E	245	ASP
1	E	364	GLU
1	F	97	LYS
1	F	152	ARG
1	F	179	LYS
1	F	245	ASP
1	F	364	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-31	HIS
1	A	-28	HIS
1	A	-27	HIS
1	A	41	GLN
1	A	250	GLN
1	A	319	GLN
1	A	321	GLN
1	B	-30	HIS
1	B	-28	HIS
1	B	250	GLN

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Mol	Chain	Res	Type
1	B	328	GLN
1	C	76	GLN
1	C	354	GLN
1	C	356	GLN
1	D	41	GLN
1	D	321	GLN
1	E	41	GLN
1	E	250	GLN
1	E	319	GLN
1	E	321	GLN
1	F	250	GLN
1	F	319	GLN
1	F	321	GLN
1	F	353	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

77 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	PEG	A	406	-	6,6,6	0.44	0	5,5,5	0.47	0
3	PEG	C	1005	-	6,6,6	0.40	0	5,5,5	0.27	0
3	PEG	B	409	-	6,6,6	0.20	0	5,5,5	0.20	0
3	PEG	F	408	-	6,6,6	0.96	1 (16%)	5,5,5	0.30	0
3	PEG	F	402	-	6,6,6	0.64	0	5,5,5	0.79	0
3	PEG	E	405	-	6,6,6	0.54	0	5,5,5	0.39	0
3	PEG	C	1006	-	6,6,6	0.50	0	5,5,5	0.81	0
3	PEG	A	408	-	6,6,6	0.37	0	5,5,5	0.51	0
3	PEG	A	413	-	6,6,6	0.13	0	5,5,5	0.10	0
3	PEG	B	414	-	6,6,6	0.32	0	5,5,5	0.33	0
3	PEG	F	412	-	6,6,6	0.48	0	5,5,5	0.59	0
3	PEG	B	405	-	6,6,6	0.78	0	5,5,5	0.37	0
3	PEG	B	411	-	6,6,6	0.38	0	5,5,5	0.33	0
3	PEG	C	1003	-	6,6,6	0.14	0	5,5,5	0.10	0
3	PEG	F	405	-	6,6,6	0.22	0	5,5,5	0.28	0
2	NAD	C	1001	-	42,48,48	0.63	0	50,73,73	0.80	3 (6%)
3	PEG	C	1008	-	6,6,6	0.31	0	5,5,5	0.29	0
3	PEG	E	406	-	6,6,6	0.31	0	5,5,5	0.53	0
3	PEG	E	402	-	6,6,6	0.49	0	5,5,5	0.63	0
3	PEG	E	410	-	6,6,6	0.17	0	5,5,5	0.09	0
3	PEG	D	405	-	6,6,6	0.33	0	5,5,5	0.50	0
3	PEG	E	404	-	6,6,6	0.23	0	5,5,5	0.26	0
3	PEG	F	409	-	6,6,6	0.45	0	5,5,5	0.25	0
2	NAD	D	401	-	42,48,48	0.63	0	50,73,73	0.80	3 (6%)
3	PEG	B	404	-	6,6,6	0.24	0	5,5,5	0.25	0
3	PEG	D	402	-	6,6,6	0.39	0	5,5,5	0.54	0
3	PEG	A	411	-	6,6,6	0.36	0	5,5,5	0.41	0
3	PEG	C	1009	-	6,6,6	0.46	0	5,5,5	0.33	0
3	PEG	B	413	-	6,6,6	0.37	0	5,5,5	0.34	0
3	PEG	F	406	-	6,6,6	0.29	0	5,5,5	0.37	0
3	PEG	E	403	-	6,6,6	0.58	0	5,5,5	0.61	0
3	PEG	C	1010	-	6,6,6	0.36	0	5,5,5	0.38	0
2	NAD	A	401	-	42,48,48	0.62	0	50,73,73	0.83	2 (4%)
3	PEG	B	403	-	6,6,6	0.91	0	5,5,5	0.38	0
3	PEG	A	403	-	6,6,6	0.44	0	5,5,5	0.62	0
3	PEG	A	407	-	6,6,6	0.35	0	5,5,5	0.21	0
3	PEG	D	404	-	6,6,6	0.47	0	5,5,5	0.45	0
3	PEG	A	402	-	6,6,6	0.40	0	5,5,5	0.59	0
3	PEG	B	408	-	6,6,6	0.59	0	5,5,5	0.51	0
3	PEG	D	406	-	6,6,6	0.84	0	5,5,5	0.39	0
3	PEG	C	1011	-	6,6,6	0.22	0	5,5,5	0.16	0
3	PEG	D	403	-	6,6,6	0.12	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	D	410	-	6,6,6	0.92	0	5,5,5	0.53	0
3	PEG	D	412	-	6,6,6	0.41	0	5,5,5	0.15	0
3	PEG	C	1004	-	6,6,6	0.37	0	5,5,5	0.30	0
2	NAD	E	401	-	42,48,48	0.61	0	50,73,73	0.85	4 (8%)
2	NAD	F	401	-	42,48,48	0.62	0	50,73,73	0.85	4 (8%)
3	PEG	E	411	-	6,6,6	0.48	0	5,5,5	0.38	0
3	PEG	B	402	-	6,6,6	0.41	0	5,5,5	0.72	0
3	PEG	D	413	-	6,6,6	0.36	0	5,5,5	0.21	0
3	PEG	B	410	-	6,6,6	0.28	0	5,5,5	0.28	0
3	PEG	C	1012	-	6,6,6	0.76	0	5,5,5	0.55	0
3	PEG	B	407	-	6,6,6	0.52	0	5,5,5	0.62	0
3	PEG	B	416	-	6,6,6	0.45	0	5,5,5	0.46	0
3	PEG	F	410	-	6,6,6	0.41	0	5,5,5	0.41	0
3	PEG	D	408	-	6,6,6	0.23	0	5,5,5	0.48	0
3	PEG	C	1002	-	6,6,6	0.33	0	5,5,5	0.26	0
3	PEG	E	409	-	6,6,6	0.51	0	5,5,5	0.50	0
3	PEG	F	404	-	6,6,6	0.98	0	5,5,5	0.33	0
3	PEG	F	411	-	6,6,6	0.30	0	5,5,5	0.16	0
3	PEG	C	1007	-	6,6,6	0.45	0	5,5,5	0.39	0
3	PEG	E	408	-	6,6,6	0.48	0	5,5,5	0.52	0
3	PEG	D	409	-	6,6,6	0.30	0	5,5,5	0.34	0
3	PEG	A	412	-	6,6,6	0.52	0	5,5,5	0.49	0
3	PEG	F	407	-	6,6,6	0.77	0	5,5,5	0.29	0
3	PEG	A	404	-	6,6,6	0.98	0	5,5,5	0.40	0
2	NAD	B	401	-	42,48,48	0.62	0	50,73,73	0.82	2 (4%)
3	PEG	F	403	-	6,6,6	0.18	0	5,5,5	0.09	0
3	PEG	D	411	-	6,6,6	0.41	0	5,5,5	0.39	0
3	PEG	B	415	-	6,6,6	0.60	0	5,5,5	0.54	0
3	PEG	A	405	-	6,6,6	0.29	0	5,5,5	0.32	0
3	PEG	B	406	-	6,6,6	0.40	0	5,5,5	0.32	0
3	PEG	B	412	-	6,6,6	0.23	0	5,5,5	0.17	0
3	PEG	E	407	-	6,6,6	0.43	0	5,5,5	0.56	0
3	PEG	A	409	-	6,6,6	0.31	0	5,5,5	0.30	0
3	PEG	A	410	-	6,6,6	0.51	0	5,5,5	0.35	0
3	PEG	D	407	-	6,6,6	0.28	0	5,5,5	0.21	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	PEG	A	406	-	-	3/4/4/4	-
3	PEG	C	1005	-	-	3/4/4/4	-
3	PEG	B	409	-	-	4/4/4/4	-
3	PEG	F	408	-	-	1/4/4/4	-
3	PEG	F	402	-	-	1/4/4/4	-
3	PEG	E	405	-	-	2/4/4/4	-
3	PEG	C	1006	-	-	3/4/4/4	-
3	PEG	A	408	-	-	1/4/4/4	-
3	PEG	A	413	-	-	1/4/4/4	-
3	PEG	B	414	-	-	0/4/4/4	-
3	PEG	F	412	-	-	2/4/4/4	-
3	PEG	B	405	-	-	1/4/4/4	-
3	PEG	B	411	-	-	1/4/4/4	-
3	PEG	C	1003	-	-	1/4/4/4	-
3	PEG	F	405	-	-	1/4/4/4	-
2	NAD	C	1001	-	-	4/26/62/62	0/5/5/5
3	PEG	C	1008	-	-	1/4/4/4	-
3	PEG	E	406	-	-	1/4/4/4	-
3	PEG	E	402	-	-	3/4/4/4	-
3	PEG	E	410	-	-	2/4/4/4	-
3	PEG	D	405	-	-	1/4/4/4	-
3	PEG	E	404	-	-	3/4/4/4	-
3	PEG	F	409	-	-	1/4/4/4	-
2	NAD	D	401	-	-	4/26/62/62	0/5/5/5
3	PEG	B	404	-	-	2/4/4/4	-
3	PEG	D	402	-	-	0/4/4/4	-
3	PEG	A	411	-	-	1/4/4/4	-
3	PEG	C	1009	-	-	1/4/4/4	-
3	PEG	B	413	-	-	2/4/4/4	-
3	PEG	F	406	-	-	2/4/4/4	-
3	PEG	E	403	-	-	2/4/4/4	-
3	PEG	C	1010	-	-	1/4/4/4	-
2	NAD	A	401	-	-	3/26/62/62	0/5/5/5
3	PEG	B	403	-	-	2/4/4/4	-
3	PEG	A	403	-	-	1/4/4/4	-
3	PEG	A	407	-	-	0/4/4/4	-
3	PEG	D	404	-	-	2/4/4/4	-
3	PEG	A	402	-	-	3/4/4/4	-
3	PEG	B	408	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	406	-	-	2/4/4/4	-
3	PEG	C	1011	-	-	1/4/4/4	-
3	PEG	D	403	-	-	0/4/4/4	-
3	PEG	D	410	-	-	1/4/4/4	-
3	PEG	D	412	-	-	3/4/4/4	-
3	PEG	C	1004	-	-	3/4/4/4	-
2	NAD	E	401	-	-	3/26/62/62	0/5/5/5
2	NAD	F	401	-	-	4/26/62/62	0/5/5/5
3	PEG	E	411	-	-	3/4/4/4	-
3	PEG	B	402	-	-	1/4/4/4	-
3	PEG	D	413	-	-	3/4/4/4	-
3	PEG	B	410	-	-	1/4/4/4	-
3	PEG	C	1012	-	-	0/4/4/4	-
3	PEG	B	407	-	-	1/4/4/4	-
3	PEG	B	416	-	-	3/4/4/4	-
3	PEG	F	410	-	-	1/4/4/4	-
3	PEG	D	408	-	-	1/4/4/4	-
3	PEG	C	1002	-	-	0/4/4/4	-
3	PEG	E	409	-	-	1/4/4/4	-
3	PEG	F	404	-	-	1/4/4/4	-
3	PEG	F	411	-	-	0/4/4/4	-
3	PEG	C	1007	-	-	1/4/4/4	-
3	PEG	E	408	-	-	1/4/4/4	-
3	PEG	D	409	-	-	2/4/4/4	-
3	PEG	A	412	-	-	2/4/4/4	-
3	PEG	F	407	-	-	2/4/4/4	-
3	PEG	A	404	-	-	2/4/4/4	-
2	NAD	B	401	-	-	3/26/62/62	0/5/5/5
3	PEG	F	403	-	-	1/4/4/4	-
3	PEG	D	411	-	-	1/4/4/4	-
3	PEG	B	415	-	-	1/4/4/4	-
3	PEG	A	405	-	-	1/4/4/4	-
3	PEG	B	406	-	-	1/4/4/4	-
3	PEG	B	412	-	-	1/4/4/4	-
3	PEG	E	407	-	-	2/4/4/4	-
3	PEG	A	409	-	-	0/4/4/4	-
3	PEG	A	410	-	-	0/4/4/4	-
3	PEG	D	407	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	408	PEG	O4-C4	2.13	1.53	1.42

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	NAD	C6N-N1N-C2N	-2.57	119.63	121.97
2	F	401	NAD	C6N-N1N-C2N	-2.53	119.67	121.97
2	F	401	NAD	C5A-C6A-N6A	2.47	124.11	120.35
2	A	401	NAD	C6N-N1N-C2N	-2.47	119.72	121.97
2	E	401	NAD	C5A-C6A-N6A	2.46	124.09	120.35
2	C	1001	NAD	C5A-C6A-N6A	2.41	124.02	120.35
2	D	401	NAD	C5A-C6A-N6A	2.36	123.94	120.35
2	B	401	NAD	C6N-N1N-C2N	-2.31	119.87	121.97
2	C	1001	NAD	C6N-N1N-C2N	-2.27	119.91	121.97
2	D	401	NAD	C6N-N1N-C2N	-2.27	119.91	121.97
2	B	401	NAD	C5A-C6A-N6A	2.24	123.76	120.35
2	A	401	NAD	C5A-C6A-N6A	2.23	123.74	120.35
2	F	401	NAD	O4D-C1D-C2D	-2.15	103.78	106.93
2	E	401	NAD	O4D-C1D-C2D	-2.14	103.79	106.93
2	E	401	NAD	O4B-C1B-C2B	-2.10	103.86	106.93
2	D	401	NAD	O4B-C1B-C2B	-2.07	103.89	106.93
2	C	1001	NAD	O4B-C1B-C2B	-2.06	103.91	106.93
2	F	401	NAD	O4B-C1B-C2B	-2.02	103.97	106.93

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	1001	NAD	O4D-C1D-N1N-C2N
2	C	1001	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
3	B	409	PEG	C4-C3-O2-C2
3	E	407	PEG	C4-C3-O2-C2
3	B	410	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	B	405	PEG	O2-C3-C4-O4
3	E	411	PEG	O2-C3-C4-O4
3	A	408	PEG	C4-C3-O2-C2
3	A	404	PEG	O2-C3-C4-O4
3	D	404	PEG	O2-C3-C4-O4
3	D	408	PEG	O2-C3-C4-O4
3	E	402	PEG	O2-C3-C4-O4
3	E	405	PEG	O2-C3-C4-O4
3	A	406	PEG	O2-C3-C4-O4
3	B	402	PEG	O2-C3-C4-O4
3	B	403	PEG	O1-C1-C2-O2
3	B	413	PEG	O2-C3-C4-O4
3	C	1004	PEG	O2-C3-C4-O4
3	D	410	PEG	O2-C3-C4-O4
3	F	402	PEG	O2-C3-C4-O4
3	F	404	PEG	O2-C3-C4-O4
3	C	1003	PEG	C1-C2-O2-C3
3	A	405	PEG	O2-C3-C4-O4
3	B	409	PEG	O1-C1-C2-O2
3	E	402	PEG	O1-C1-C2-O2
3	E	410	PEG	O1-C1-C2-O2
3	D	412	PEG	C1-C2-O2-C3
3	A	406	PEG	O1-C1-C2-O2
3	B	415	PEG	O1-C1-C2-O2
3	F	405	PEG	O1-C1-C2-O2
3	B	416	PEG	O2-C3-C4-O4
3	D	406	PEG	C4-C3-O2-C2
3	B	416	PEG	C4-C3-O2-C2
3	A	403	PEG	O1-C1-C2-O2
3	A	412	PEG	O2-C3-C4-O4
3	C	1005	PEG	O1-C1-C2-O2
3	C	1005	PEG	O2-C3-C4-O4
3	C	1006	PEG	O2-C3-C4-O4
3	D	407	PEG	O1-C1-C2-O2
3	E	407	PEG	O2-C3-C4-O4
3	C	1004	PEG	C4-C3-O2-C2
3	F	412	PEG	C4-C3-O2-C2
3	B	411	PEG	O1-C1-C2-O2
3	C	1004	PEG	O1-C1-C2-O2
3	E	403	PEG	O1-C1-C2-O2
3	F	406	PEG	O1-C1-C2-O2
3	A	413	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	E	411	PEG	C1-C2-O2-C3
3	D	409	PEG	C1-C2-O2-C3
3	A	404	PEG	O1-C1-C2-O2
3	D	407	PEG	O2-C3-C4-O4
3	A	406	PEG	C4-C3-O2-C2
3	D	413	PEG	O2-C3-C4-O4
3	E	403	PEG	C4-C3-O2-C2
3	E	402	PEG	C1-C2-O2-C3
3	A	402	PEG	O2-C3-C4-O4
3	D	405	PEG	O1-C1-C2-O2
3	B	408	PEG	C1-C2-O2-C3
3	B	403	PEG	C4-C3-O2-C2
3	A	411	PEG	C4-C3-O2-C2
3	B	407	PEG	O1-C1-C2-O2
3	B	409	PEG	O2-C3-C4-O4
3	D	412	PEG	O2-C3-C4-O4
3	B	413	PEG	C4-C3-O2-C2
3	F	410	PEG	C4-C3-O2-C2
3	D	413	PEG	C4-C3-O2-C2
3	E	404	PEG	O1-C1-C2-O2
3	E	409	PEG	C1-C2-O2-C3
3	B	412	PEG	O2-C3-C4-O4
3	F	408	PEG	O2-C3-C4-O4
3	F	412	PEG	O2-C3-C4-O4
3	C	1006	PEG	C1-C2-O2-C3
3	C	1011	PEG	C4-C3-O2-C2
3	B	404	PEG	O1-C1-C2-O2
3	B	406	PEG	O1-C1-C2-O2
3	E	411	PEG	O1-C1-C2-O2
3	F	409	PEG	O2-C3-C4-O4
3	D	413	PEG	C1-C2-O2-C3
3	B	416	PEG	C1-C2-O2-C3
3	D	406	PEG	O1-C1-C2-O2
3	F	406	PEG	C4-C3-O2-C2
3	D	407	PEG	C1-C2-O2-C3
3	C	1009	PEG	C1-C2-O2-C3
3	E	404	PEG	C1-C2-O2-C3
3	B	409	PEG	C1-C2-O2-C3
3	D	409	PEG	C4-C3-O2-C2
3	D	412	PEG	O1-C1-C2-O2
3	B	404	PEG	C4-C3-O2-C2
3	C	1010	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	B	408	PEG	C4-C3-O2-C2
3	A	402	PEG	C4-C3-O2-C2
3	E	410	PEG	C1-C2-O2-C3
3	C	1007	PEG	C4-C3-O2-C2
3	A	412	PEG	C1-C2-O2-C3
3	E	406	PEG	C1-C2-O2-C3
2	A	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	C	1001	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	E	401	NAD	C2D-C1D-N1N-C2N
3	C	1008	PEG	O2-C3-C4-O4
3	E	405	PEG	C1-C2-O2-C3
2	A	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	O4B-C4B-C5B-O5B
3	F	407	PEG	C4-C3-O2-C2
3	F	407	PEG	O1-C1-C2-O2
2	C	1001	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	O4B-C4B-C5B-O5B
2	E	401	NAD	O4B-C4B-C5B-O5B
3	C	1005	PEG	C4-C3-O2-C2
3	C	1006	PEG	C4-C3-O2-C2
3	E	408	PEG	C4-C3-O2-C2
3	D	411	PEG	C1-C2-O2-C3
3	D	404	PEG	O1-C1-C2-O2
3	E	404	PEG	O2-C3-C4-O4
3	F	403	PEG	O1-C1-C2-O2
3	A	402	PEG	C1-C2-O2-C3

There are no ring outliers.

44 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	PEG	2	0
3	C	1005	PEG	2	0
3	B	409	PEG	1	0
3	C	1006	PEG	2	0
3	A	408	PEG	2	0
3	A	413	PEG	2	0
3	F	412	PEG	2	0
3	B	411	PEG	1	0

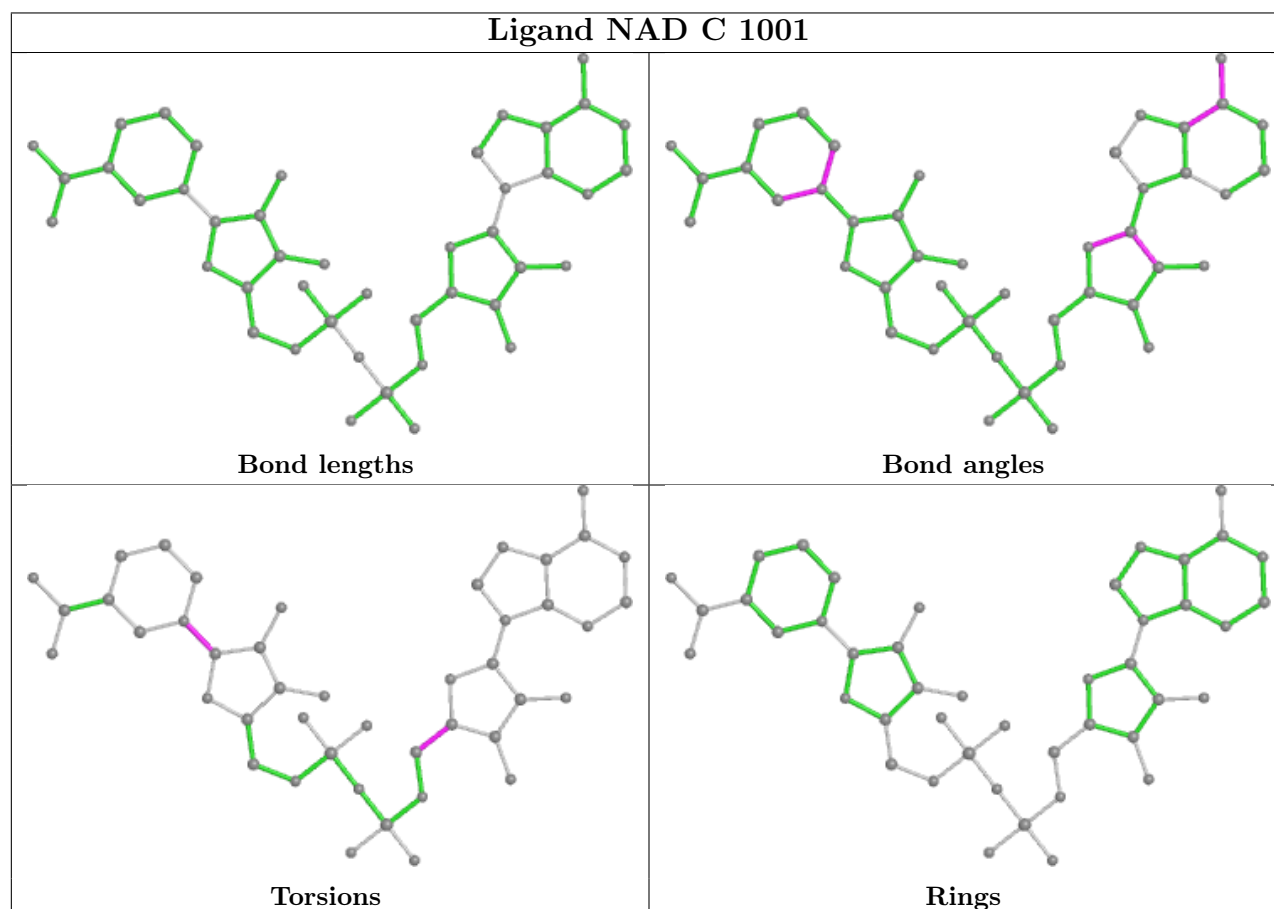
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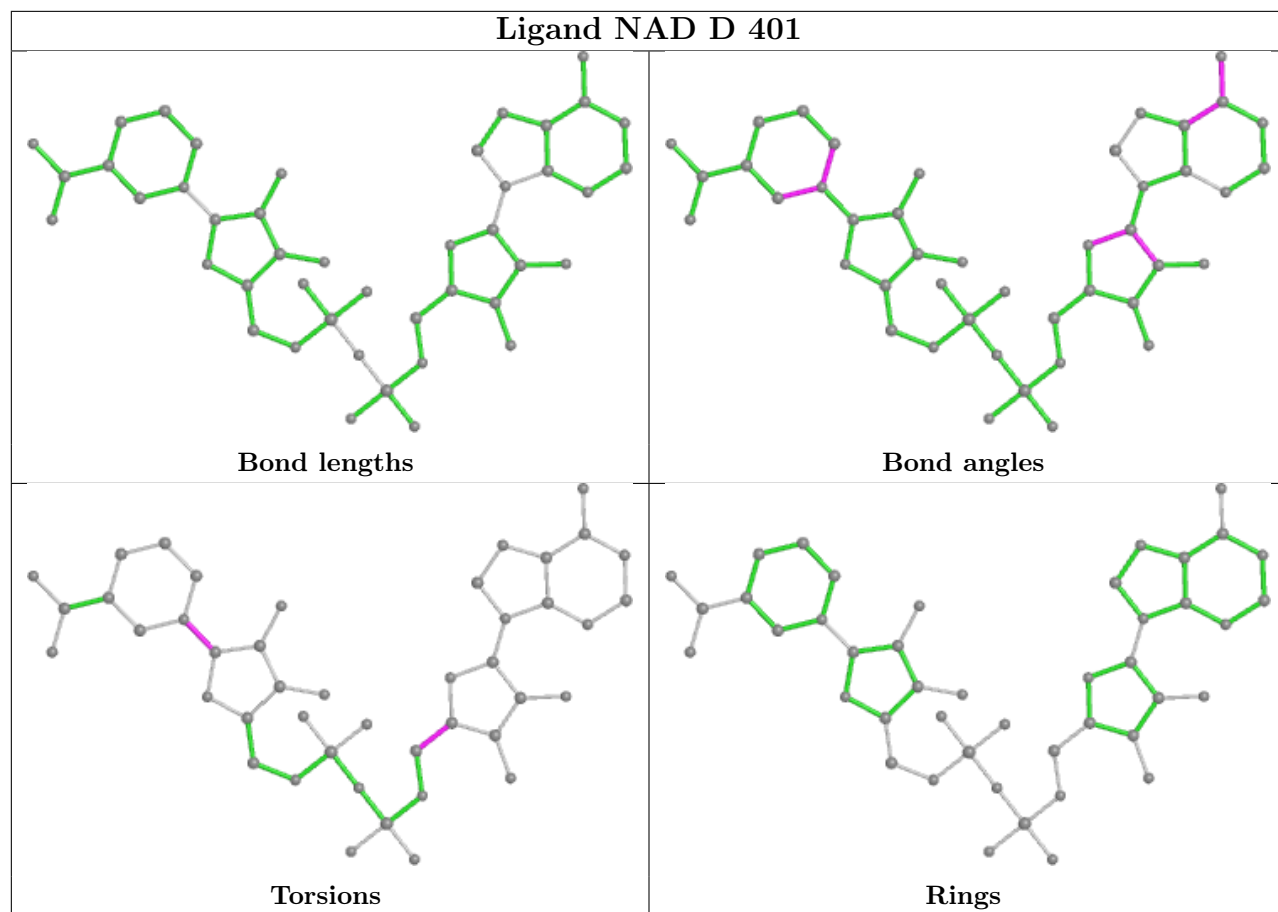
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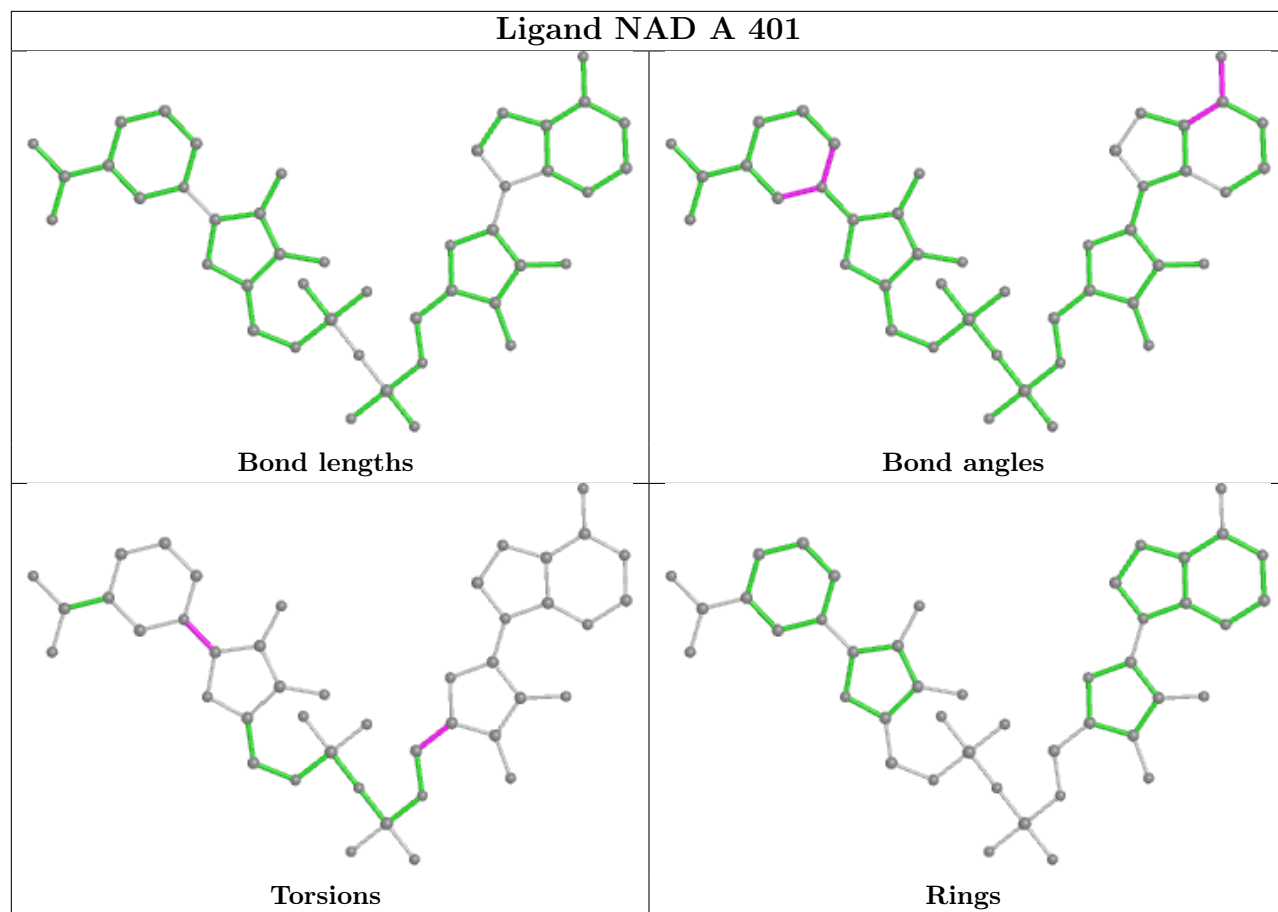
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1003	PEG	5	0
2	C	1001	NAD	1	0
3	E	406	PEG	2	0
3	E	402	PEG	3	0
3	D	405	PEG	1	0
2	D	401	NAD	1	0
3	B	404	PEG	2	0
3	D	402	PEG	2	0
3	A	411	PEG	1	0
3	C	1009	PEG	5	0
3	F	406	PEG	2	0
3	E	403	PEG	1	0
3	C	1010	PEG	2	0
2	A	401	NAD	1	0
3	A	403	PEG	2	0
3	D	404	PEG	3	0
3	B	408	PEG	1	0
3	C	1011	PEG	1	0
3	D	412	PEG	1	0
3	C	1004	PEG	5	0
2	E	401	NAD	1	0
2	F	401	NAD	2	0
3	E	411	PEG	1	0
3	B	402	PEG	3	0
3	D	413	PEG	1	0
3	C	1012	PEG	2	0
3	F	410	PEG	1	0
3	D	408	PEG	1	0
3	E	409	PEG	4	0
3	F	407	PEG	1	0
3	A	404	PEG	1	0
3	F	403	PEG	2	0
3	D	411	PEG	1	0
3	B	415	PEG	1	0
3	A	410	PEG	1	0
3	D	407	PEG	1	0

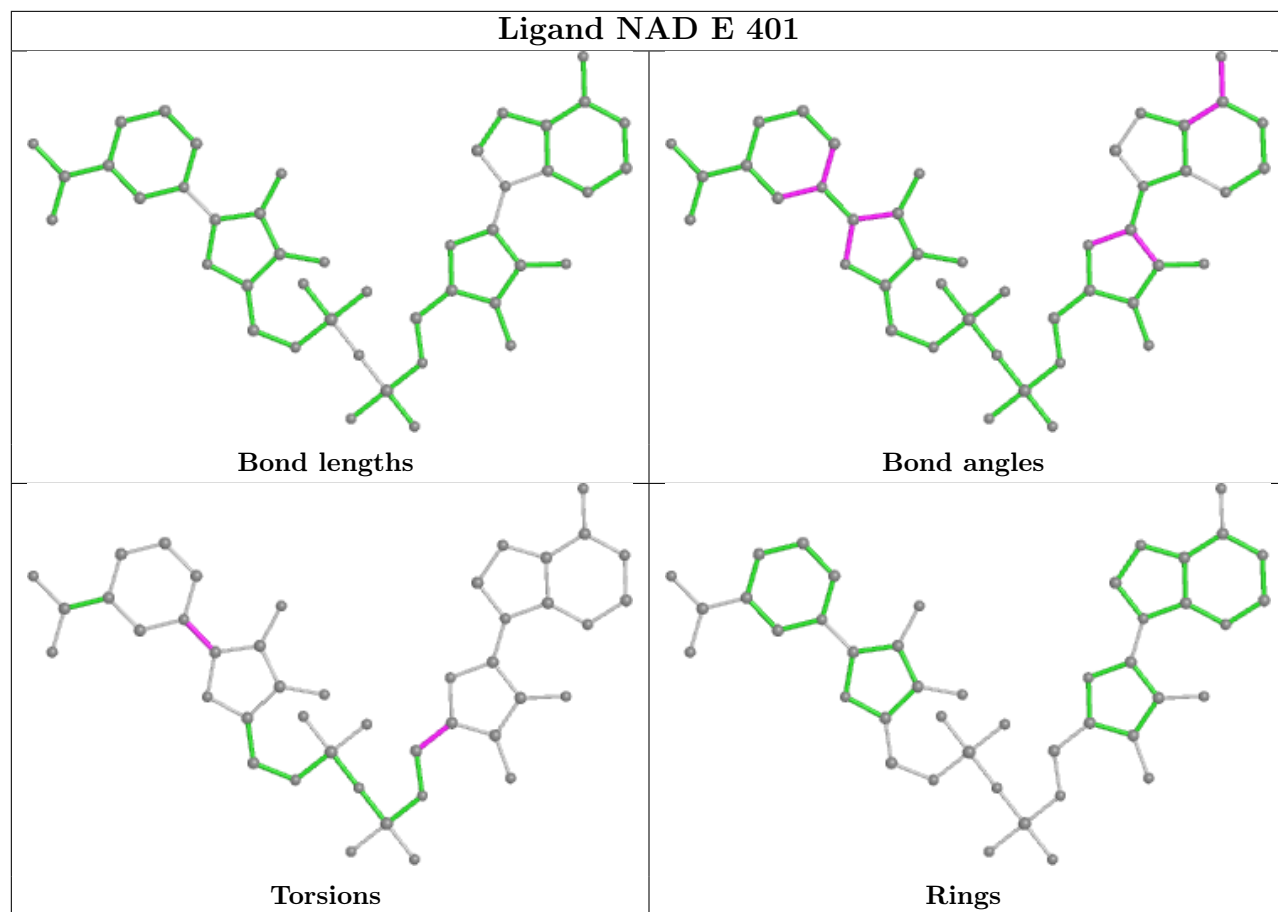
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

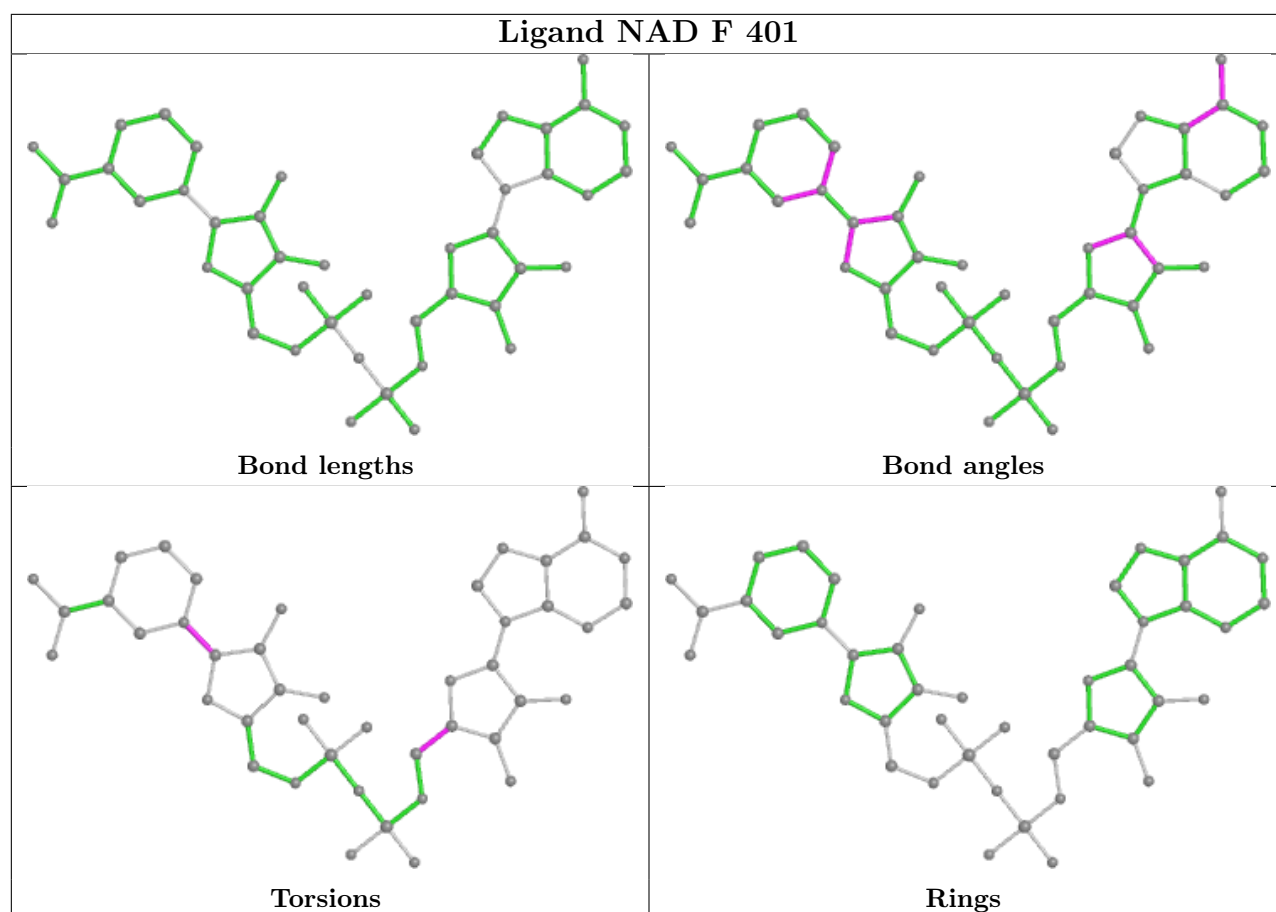
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

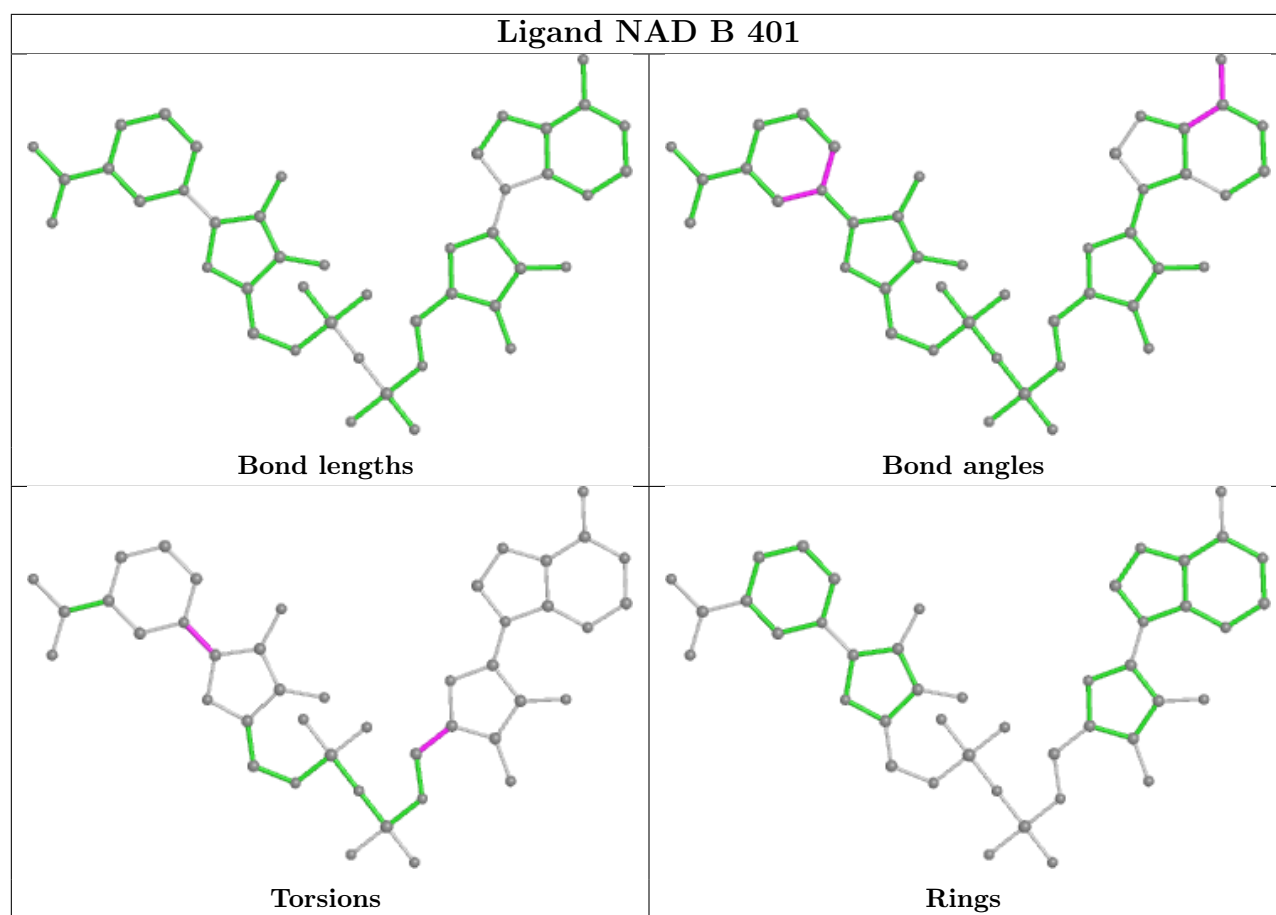












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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, 95th 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	377/400 (94%)	-0.37	13 (3%)	48	46	7, 17, 38, 81	3 (0%)
1	B	376/400 (94%)	-0.38	15 (3%)	43	40	7, 17, 38, 68	4 (1%)
1	C	363/400 (90%)	-0.33	9 (2%)	58	57	9, 18, 35, 81	4 (1%)
1	D	363/400 (90%)	-0.32	9 (2%)	58	57	9, 18, 35, 75	4 (1%)
1	E	362/400 (90%)	-0.32	5 (1%)	73	72	12, 19, 37, 67	2 (0%)
1	F	362/400 (90%)	-0.33	6 (1%)	69	67	12, 19, 37, 70	3 (0%)
All	All	2203/2400 (91%)	-0.34	57 (2%)	57	55	7, 18, 38, 81	20 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	GLY	7.5
1	F	3	LEU	6.5
1	E	3	LEU	5.8
1	C	3	LEU	5.2
1	B	364	GLU	4.6
1	D	3	LEU	4.5
1	B	210	ASP	4.4
1	E	332	THR	3.6
1	A	214	ASP	3.5
1	C	312	LEU	3.2
1	B	276	ASP	3.2
1	A	111	GLN	3.2
1	A	-34	GLY	3.2
1	A	-21	VAL	3.1
1	B	214	ASP	3.1
1	B	-21	VAL	3.0
1	C	313	GLY	3.0
1	D	214	ASP	3.0
1	B	111	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	333	GLU	2.9
1	D	277	LEU	2.9
1	B	-29	HIS	2.8
1	A	276	ASP	2.7
1	A	-29	HIS	2.7
1	B	-22	LEU	2.7
1	B	-34	GLY	2.7
1	F	333	GLU	2.6
1	F	332	THR	2.5
1	C	399	GLU	2.5
1	A	275	GLY	2.5
1	A	277	LEU	2.4
1	D	364	GLU	2.4
1	A	-22	LEU	2.4
1	C	314	ALA	2.4
1	D	278	GLY	2.4
1	A	3	LEU	2.3
1	B	330	SER	2.3
1	B	291	LEU	2.3
1	F	364	GLU	2.3
1	E	364	GLU	2.3
1	B	277	LEU	2.2
1	D	2	GLN	2.2
1	A	-26	HIS	2.2
1	F	214	ASP	2.2
1	C	340	LYS	2.2
1	C	2	GLN	2.1
1	D	279	ALA	2.1
1	C	309	PRO	2.1
1	C	249	ASP	2.1
1	B	275	GLY	2.1
1	B	-26	HIS	2.1
1	A	5	ARG	2.1
1	D	274	PRO	2.0
1	B	3	LEU	2.0
1	E	276	ASP	2.0
1	F	26	ASP	2.0
1	D	38	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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(\AA^2)	Q<0.9
3	PEG	C	1006	7/7	0.53	0.27	59,72,84,86	0
3	PEG	E	411	7/7	0.56	0.23	48,56,76,79	0
3	PEG	D	412	7/7	0.57	0.20	59,60,65,67	0
3	PEG	D	409	7/7	0.57	0.25	56,71,92,98	0
3	PEG	B	410	7/7	0.61	0.23	54,60,70,84	0
3	PEG	C	1007	7/7	0.62	0.22	54,58,85,89	0
3	PEG	B	407	7/7	0.64	0.28	52,60,70,76	0
3	PEG	A	407	7/7	0.64	0.20	44,57,80,92	0
3	PEG	D	408	7/7	0.64	0.23	57,76,80,85	0
3	PEG	D	411	7/7	0.65	0.26	65,73,83,89	0
3	PEG	E	409	7/7	0.66	0.27	54,70,81,83	0
3	PEG	C	1008	7/7	0.67	0.25	58,60,76,83	0
3	PEG	B	412	7/7	0.68	0.19	49,57,66,71	0
3	PEG	A	413	7/7	0.68	0.21	41,48,59,66	0
3	PEG	D	403	7/7	0.68	0.22	37,44,49,61	0
3	PEG	C	1004	7/7	0.69	0.21	38,46,51,51	0
3	PEG	F	407	7/7	0.69	0.21	43,45,58,75	0
3	PEG	B	409	7/7	0.70	0.24	58,61,83,87	0
3	PEG	E	408	7/7	0.71	0.21	49,59,66,70	0
3	PEG	A	405	7/7	0.71	0.18	51,61,70,70	0
3	PEG	D	406	7/7	0.71	0.17	41,47,55,77	0
3	PEG	F	406	7/7	0.71	0.28	64,77,85,89	0
3	PEG	B	414	7/7	0.71	0.26	62,65,82,84	0
3	PEG	F	409	7/7	0.71	0.19	48,54,65,69	0
3	PEG	F	410	7/7	0.71	0.20	49,55,88,96	0
3	PEG	D	410	7/7	0.72	0.20	35,44,62,72	0
3	PEG	E	404	7/7	0.72	0.21	44,53,63,77	0
3	PEG	C	1003	7/7	0.72	0.23	35,43,58,66	0
3	PEG	B	411	7/7	0.74	0.22	53,57,72,79	0
3	PEG	A	404	7/7	0.75	0.23	45,48,77,79	0
3	PEG	F	412	7/7	0.75	0.22	44,49,63,65	0
3	PEG	B	416	7/7	0.76	0.20	43,58,64,64	0

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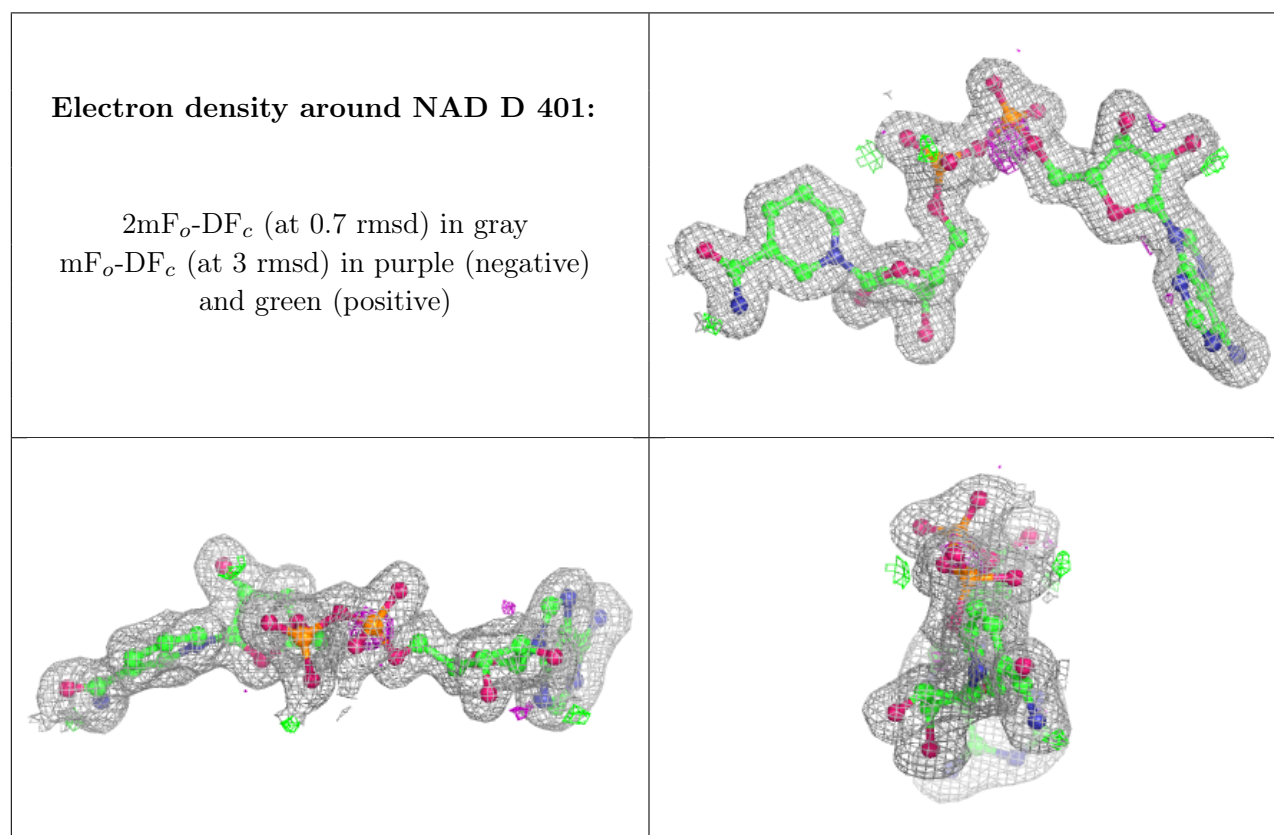
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEG	E	410	7/7	0.76	0.21	46,54,68,74	0
3	PEG	A	408	7/7	0.76	0.22	53,58,68,75	0
3	PEG	B	406	7/7	0.76	0.22	48,53,55,59	0
3	PEG	F	403	7/7	0.77	0.21	36,44,48,51	0
3	PEG	A	410	7/7	0.77	0.18	45,54,56,66	0
3	PEG	C	1009	7/7	0.77	0.19	34,46,52,61	0
3	PEG	C	1010	7/7	0.77	0.16	48,50,58,58	0
3	PEG	A	406	7/7	0.77	0.22	40,46,63,71	0
3	PEG	B	413	7/7	0.77	0.22	53,56,80,83	0
3	PEG	A	403	7/7	0.78	0.22	29,39,53,57	0
3	PEG	F	404	7/7	0.78	0.20	39,41,48,53	0
3	PEG	F	405	7/7	0.78	0.19	48,54,56,59	0
3	PEG	C	1012	7/7	0.78	0.18	40,43,47,61	0
3	PEG	D	413	7/7	0.79	0.18	35,45,52,57	0
3	PEG	E	405	7/7	0.79	0.17	42,50,56,65	0
3	PEG	B	402	7/7	0.80	0.23	30,34,46,50	0
3	PEG	C	1005	7/7	0.80	0.16	45,51,53,69	0
3	PEG	E	402	7/7	0.80	0.17	34,35,39,46	0
3	PEG	F	411	7/7	0.80	0.18	40,46,74,75	0
3	PEG	F	402	7/7	0.80	0.29	38,45,50,54	0
3	PEG	D	407	7/7	0.81	0.16	43,49,53,73	0
3	PEG	D	404	7/7	0.81	0.17	38,42,54,57	0
3	PEG	E	406	7/7	0.81	0.15	33,40,45,47	0
3	PEG	E	407	7/7	0.81	0.20	40,53,69,70	0
3	PEG	D	405	7/7	0.81	0.17	44,50,57,58	0
3	PEG	C	1002	7/7	0.81	0.16	35,37,42,43	0
3	PEG	B	408	7/7	0.82	0.18	46,57,66,69	0
3	PEG	A	411	7/7	0.82	0.14	25,33,41,42	0
3	PEG	B	404	7/7	0.82	0.16	32,37,51,54	0
3	PEG	B	403	7/7	0.83	0.19	35,42,49,56	0
3	PEG	C	1011	7/7	0.83	0.14	38,47,55,64	0
3	PEG	A	412	7/7	0.83	0.18	40,43,50,50	0
3	PEG	D	402	7/7	0.84	0.21	38,42,46,54	0
3	PEG	E	403	7/7	0.85	0.16	40,43,48,51	0
3	PEG	F	408	7/7	0.85	0.13	30,34,46,51	0
3	PEG	A	409	7/7	0.86	0.13	41,47,52,55	0
3	PEG	A	402	7/7	0.86	0.13	28,31,33,35	0
3	PEG	B	405	7/7	0.86	0.15	33,37,59,59	0
3	PEG	B	415	7/7	0.88	0.12	25,30,42,43	0
2	NAD	D	401	44/44	0.97	0.06	13,18,22,23	0
2	NAD	C	1001	44/44	0.97	0.06	13,18,22,23	0
2	NAD	F	401	44/44	0.98	0.04	11,16,19,21	0

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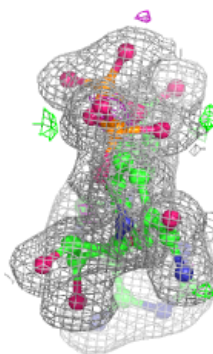
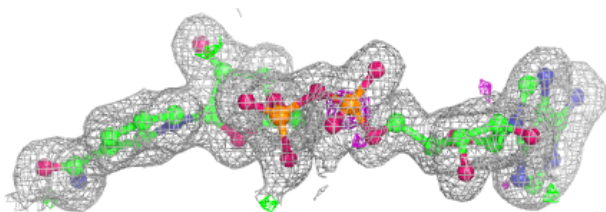
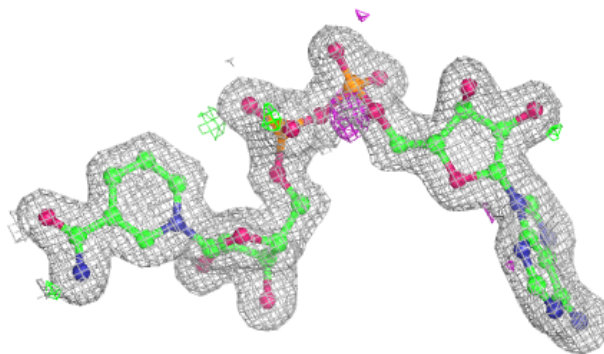
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	A	401	44/44	0.98	0.05	9,13,16,21	0
2	NAD	B	401	44/44	0.98	0.04	11,13,16,21	0
2	NAD	E	401	44/44	0.98	0.05	11,16,19,21	0

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.

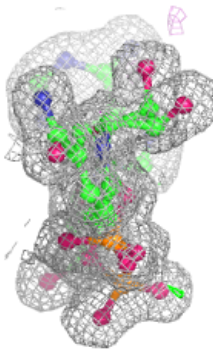
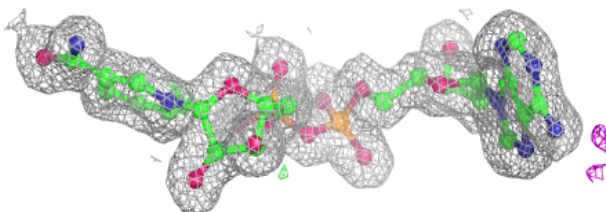
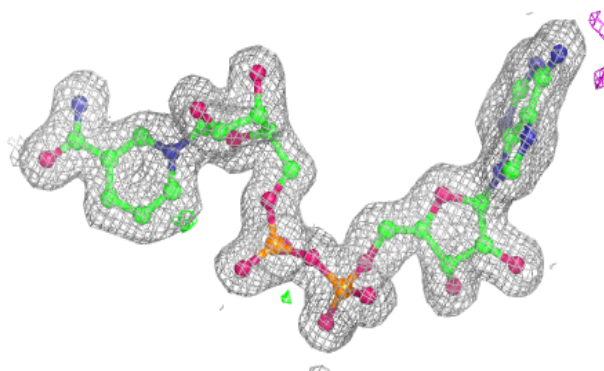


Electron density around NAD C 1001:

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

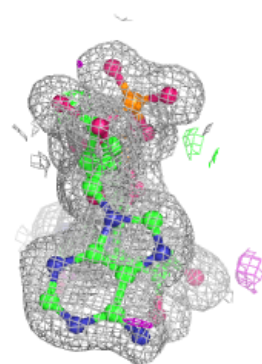
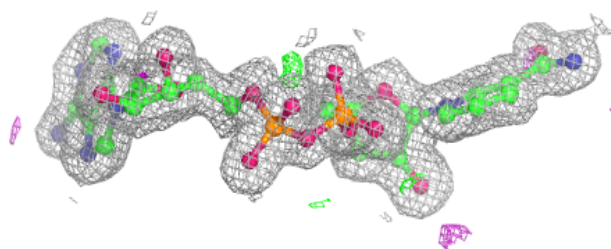
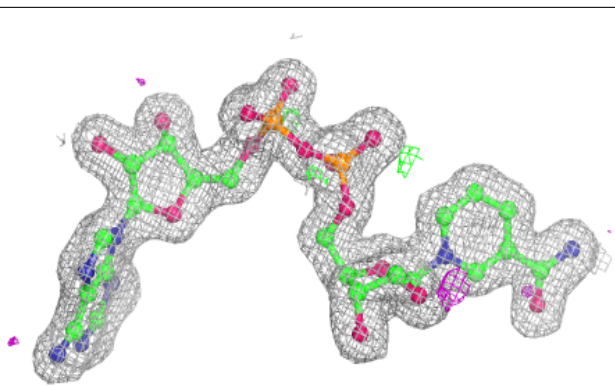
**Electron density around NAD F 401:**

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

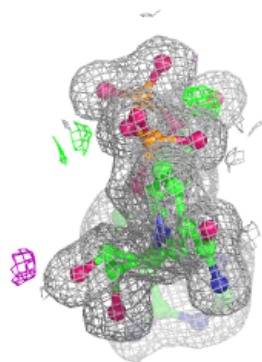
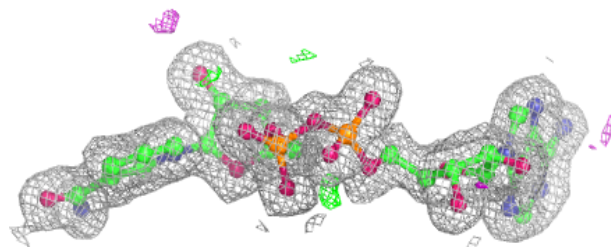
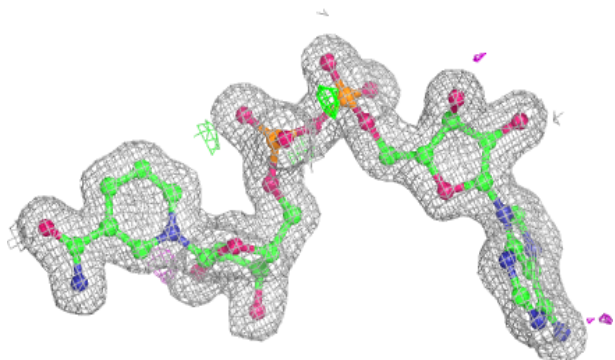


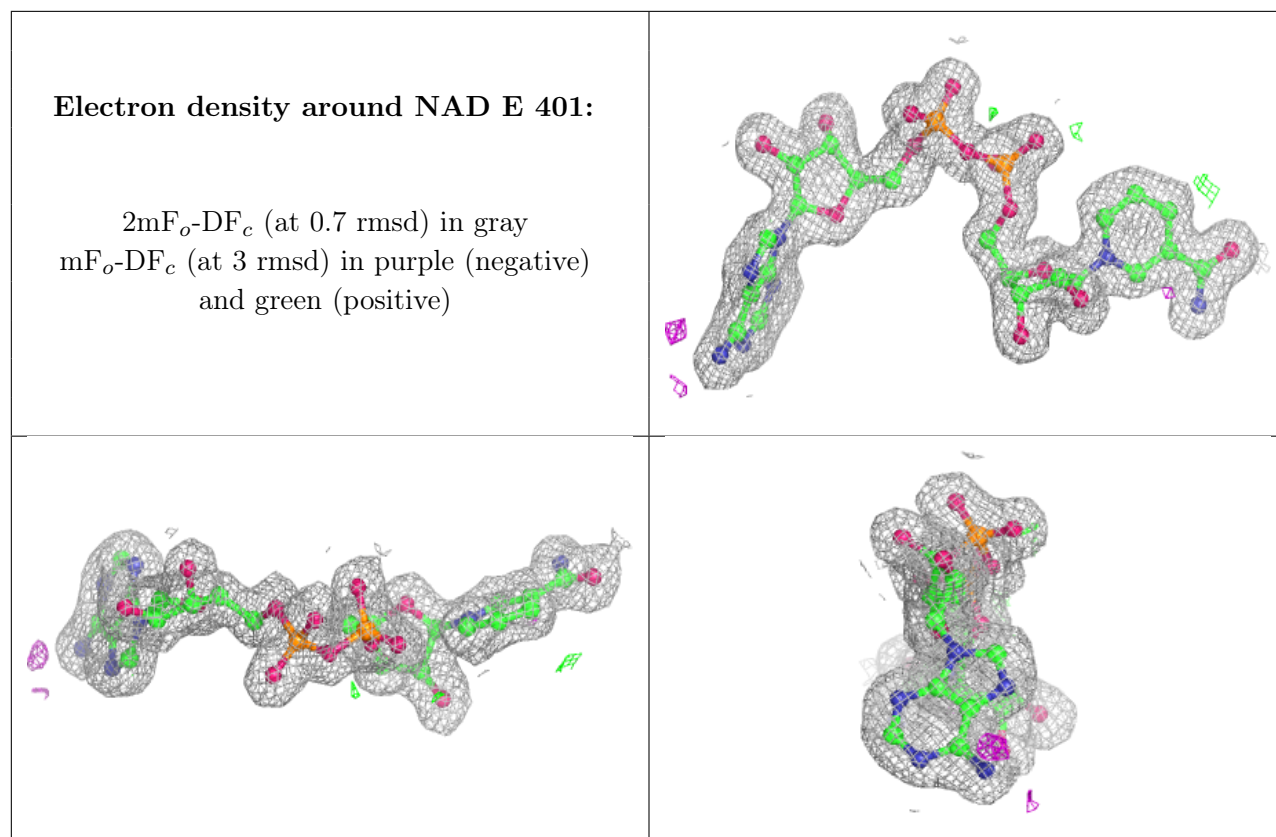
Electron density around NAD A 401:

$2mF_o-DF_c$ (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.