



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 08:41 PM EDT

PDB ID : 6IXN  
Title : Crystal structure of isocitrate dehydrogenase from *Ostreococcus tauri* in complex with NAD<sup>+</sup> and citrate  
Authors : Zhu, G.P.; Tang, W.G.; Wang, P.  
Deposited on : 2018-12-11  
Resolution : 1.87 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

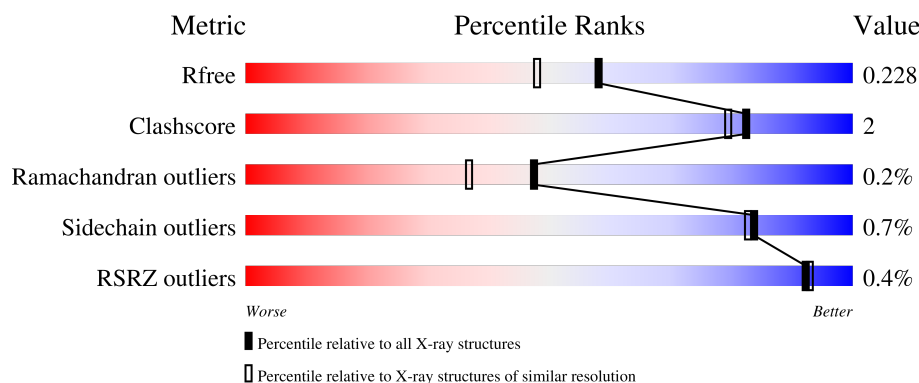
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


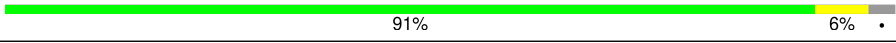
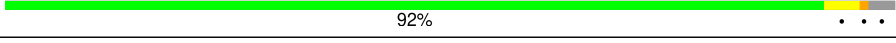

The reported resolution of this entry is 1.87 Å.

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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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  $\geq 3$ , 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	418	
1	B	418	
1	C	418	
1	D	418	

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
4	FLC	D	505	-	X	-	-
6	PEG	B	504	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14179 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 Isocitrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3172	1998	561	599	14			
1	B	405	Total	C	N	O	S	0	0	0
			3155	1987	553	601	14			
1	C	405	Total	C	N	O	S	0	0	0
			3164	1993	556	601	14			
1	D	405	Total	C	N	O	S	0	0	0
			3167	1995	557	601	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A0A1Y5IEA9
A	13	HIS	-	expression tag	UNP A0A1Y5IEA9
A	14	HIS	-	expression tag	UNP A0A1Y5IEA9
A	15	HIS	-	expression tag	UNP A0A1Y5IEA9
A	16	HIS	-	expression tag	UNP A0A1Y5IEA9
A	17	HIS	-	expression tag	UNP A0A1Y5IEA9
A	18	HIS	-	expression tag	UNP A0A1Y5IEA9
A	19	HIS	-	expression tag	UNP A0A1Y5IEA9
B	12	GLY	-	expression tag	UNP A0A1Y5IEA9
B	13	HIS	-	expression tag	UNP A0A1Y5IEA9
B	14	HIS	-	expression tag	UNP A0A1Y5IEA9
B	15	HIS	-	expression tag	UNP A0A1Y5IEA9
B	16	HIS	-	expression tag	UNP A0A1Y5IEA9
B	17	HIS	-	expression tag	UNP A0A1Y5IEA9
B	18	HIS	-	expression tag	UNP A0A1Y5IEA9
B	19	HIS	-	expression tag	UNP A0A1Y5IEA9
C	12	GLY	-	expression tag	UNP A0A1Y5IEA9
C	13	HIS	-	expression tag	UNP A0A1Y5IEA9
C	14	HIS	-	expression tag	UNP A0A1Y5IEA9
C	15	HIS	-	expression tag	UNP A0A1Y5IEA9
C	16	HIS	-	expression tag	UNP A0A1Y5IEA9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	HIS	-	expression tag	UNP A0A1Y5IEA9
C	18	HIS	-	expression tag	UNP A0A1Y5IEA9
C	19	HIS	-	expression tag	UNP A0A1Y5IEA9
D	12	GLY	-	expression tag	UNP A0A1Y5IEA9
D	13	HIS	-	expression tag	UNP A0A1Y5IEA9
D	14	HIS	-	expression tag	UNP A0A1Y5IEA9
D	15	HIS	-	expression tag	UNP A0A1Y5IEA9
D	16	HIS	-	expression tag	UNP A0A1Y5IEA9
D	17	HIS	-	expression tag	UNP A0A1Y5IEA9
D	18	HIS	-	expression tag	UNP A0A1Y5IEA9
D	19	HIS	-	expression tag	UNP A0A1Y5IEA9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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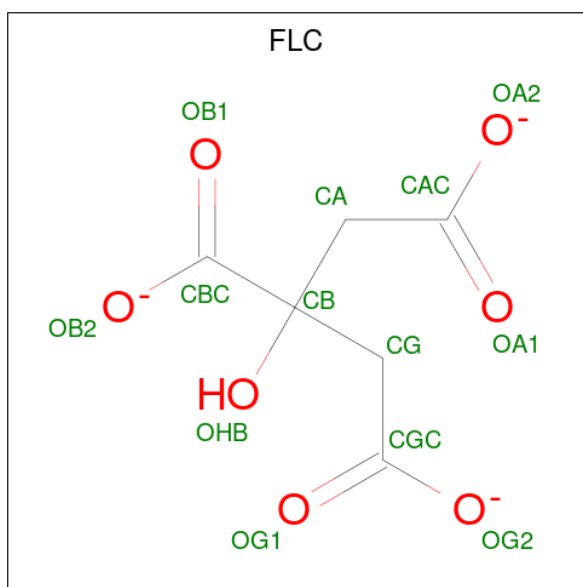
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



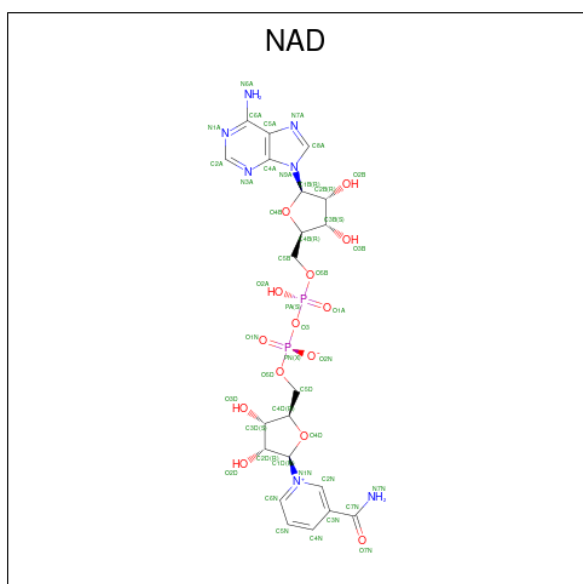
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



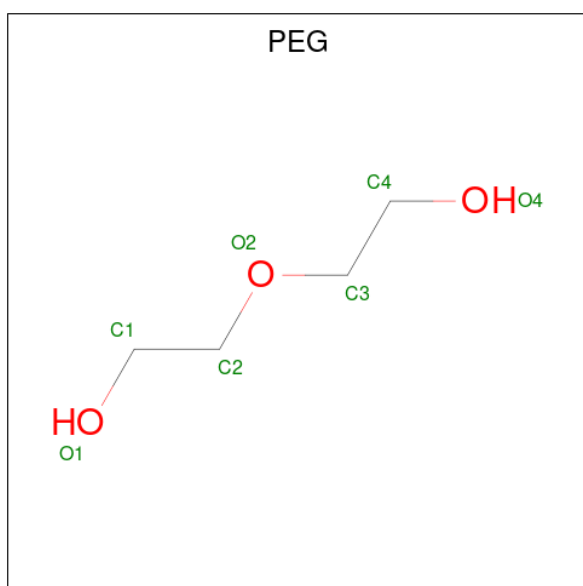
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 13	C 6	O 7	0	0
4	B	1	Total 13	C 6	O 7	0	0
4	C	1	Total 13	C 6	O 7	0	0
4	D	1	Total 13	C 6	O 7	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 7 is water.

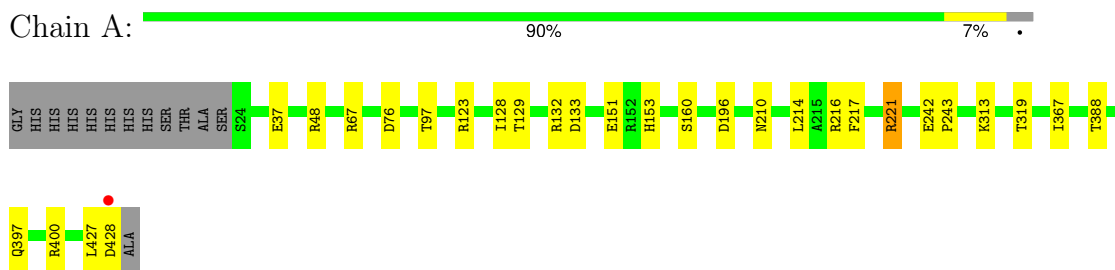
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	305	Total	O	0	0
			305	305		
7	B	302	Total	O	0	0
			302	302		
7	C	300	Total	O	0	0
			300	300		
7	D	309	Total	O	0	0
			309	309		



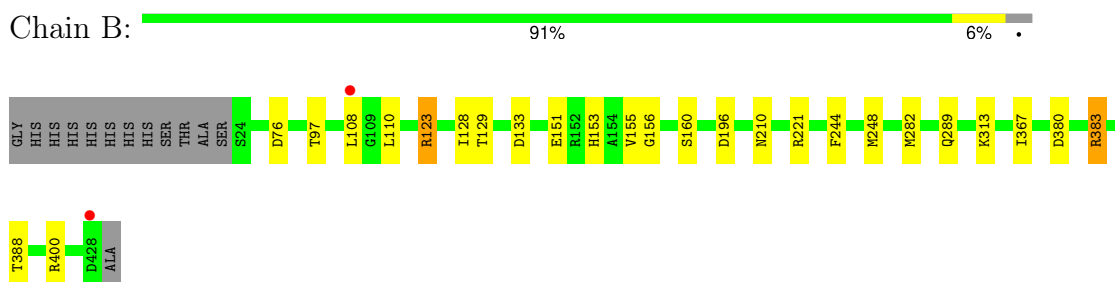
### 3 Residue-property plots [i](#)

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.

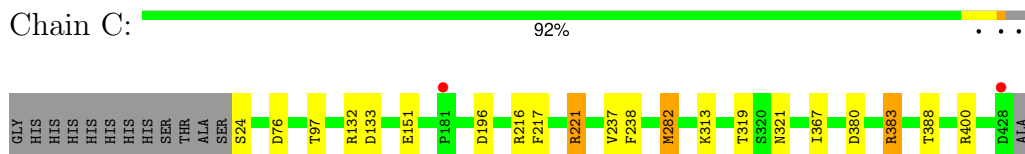
- Molecule 1: Isocitrate dehydrogenase



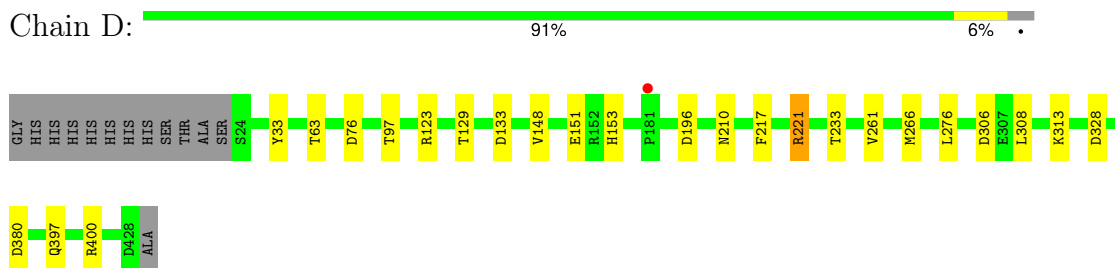
- Molecule 1: Isocitrate dehydrogenase



- Molecule 1: Isocitrate dehydrogenase



- Molecule 1: Isocitrate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.11Å 102.93Å 103.29Å 90.00° 104.07° 90.00°	Depositor
Resolution (Å)	20.00 – 1.87 19.99 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-1.87) 99.4 (19.99-1.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.195 , 0.222 0.203 , 0.228	Depositor DCC
$R_{free}$ test set	8559 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.4	Xtriage
Anisotropy	0.986	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.57$ , $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.083 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	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 45.53 % 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 1.3047e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, PEG, NAD, FLC

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	0.53	1/3239 (0.0%)	0.77	6/4383 (0.1%)
1	B	0.50	0/3222	0.75	5/4364 (0.1%)
1	C	0.48	0/3231	0.77	8/4374 (0.2%)
1	D	0.49	0/3234	0.77	6/4378 (0.1%)
All	All	0.50	1/12926 (0.0%)	0.77	25/17499 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	SER	CB-OG	7.38	1.51	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	C	221	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	A	221	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	D	221	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	221	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	221	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	400	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	400	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	C	383	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	383	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	C	400	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	C	383	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	400	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	123	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	216	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	383	ARG	NE-CZ-NH2	-5.83	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	400	ARG	CG-CD-NE	-5.56	100.13	111.80
1	D	400	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	123	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	216	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	123	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	400	ARG	CG-CD-NE	-5.16	100.97	111.80
1	C	282	MET	CG-SD-CE	-5.13	91.99	100.20
1	D	328	ASP	CB-CG-OD1	5.05	122.85	118.30

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	3172	0	3100	16	0
1	B	3155	0	3055	22	0
1	C	3164	0	3081	12	0
1	D	3167	0	3084	12	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
4	A	13	0	5	0	0
4	B	13	0	5	1	0
4	C	13	0	5	1	0
4	D	13	0	5	1	0
5	A	44	0	26	2	0
5	B	44	0	26	2	0
5	C	44	0	26	2	0
5	D	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	7	0	10	10	0
7	A	305	0	0	2	0
7	B	302	0	0	1	0
7	C	300	0	0	2	0
7	D	309	0	0	0	0
All	All	14179	0	12494	63	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 2.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ASP:OD2	1:C:221:ARG:NH2	2.09	0.85
1:A:133:ASP:OD2	1:A:221:ARG:NH2	2.09	0.84
1:D:133:ASP:OD2	1:D:221:ARG:NH2	2.18	0.76
1:B:123:ARG:HD3	6:B:504:PEG:H21	1.76	0.68
1:C:133:ASP:CG	1:C:221:ARG:HH22	1.99	0.66
1:C:24:SER:N	7:C:601:HOH:O	2.30	0.65
1:A:397:GLN:HE22	1:D:397:GLN:HE22	1.43	0.64
1:A:217:PHE:CE2	1:A:221:ARG:HD2	2.34	0.63
1:C:380:ASP:OD1	1:C:383:ARG:HD3	2.02	0.59
1:C:217:PHE:CE2	1:C:221:ARG:HD2	2.37	0.59
4:D:505:FLC:HA2	5:D:506:NAD:C4N	2.33	0.58
1:A:151:GLU:OE2	1:A:221:ARG:NH1	2.35	0.57
1:A:133:ASP:CG	1:A:221:ARG:HH22	2.08	0.56
1:C:367:ILE:HG23	1:C:388:THR:HB	1.87	0.56
1:D:133:ASP:CG	1:D:221:ARG:HH22	2.09	0.55
1:B:155:VAL:HA	6:B:504:PEG:H12	1.88	0.55
1:B:123:ARG:CG	6:B:504:PEG:H21	2.36	0.54
1:B:123:ARG:HG2	6:B:504:PEG:H21	1.90	0.54
1:A:153:HIS:HE1	1:A:210:ASN:OD1	1.91	0.54
1:C:151:GLU:OE2	1:C:221:ARG:NH1	2.38	0.54
1:A:128:ILE:HG22	1:A:129:THR:HG23	1.91	0.53
1:A:97:THR:O	5:A:505:NAD:H2N	2.09	0.53
1:B:123:ARG:CD	6:B:504:PEG:H21	2.38	0.53
1:D:217:PHE:CE2	1:D:221:ARG:HD2	2.45	0.52
1:B:133:ASP:OD2	1:B:221:ARG:NH1	2.42	0.50
1:B:367:ILE:HG23	1:B:388:THR:HB	1.93	0.50
1:B:380:ASP:OD1	1:B:383:ARG:HD3	2.11	0.50
1:B:97:THR:O	5:B:506:NAD:H2N	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLY:H	6:B:504:PEG:C1	2.24	0.49
1:B:160:SER:CB	6:B:504:PEG:H22	2.44	0.48
1:D:33:TYR:HB3	1:D:63:THR:HG22	1.94	0.48
1:D:153:HIS:HE1	1:D:210:ASN:OD1	1.96	0.48
1:C:237:VAL:HG23	1:C:238:PHE:CD1	2.48	0.48
5:A:505:NAD:H51A	1:B:282:MET:HE1	1.96	0.47
1:B:160:SER:OG	6:B:504:PEG:H22	2.14	0.47
1:D:97:THR:O	5:D:506:NAD:H2N	2.14	0.47
1:D:129:THR:OG1	1:D:151:GLU:HG3	2.15	0.46
1:B:123:ARG:HD3	6:B:504:PEG:C2	2.44	0.46
4:B:505:FLC:HG1	5:B:506:NAD:C4N	2.45	0.46
1:B:221:ARG:HD2	7:B:809:HOH:O	2.15	0.46
1:B:289:GLN:NE2	3:B:503:GOL:O2	2.49	0.46
1:A:132:ARG:HA	1:A:319:THR:O	2.16	0.45
1:B:160:SER:HB3	6:B:504:PEG:H22	1.98	0.45
1:B:153:HIS:HE1	1:B:210:ASN:OD1	1.99	0.45
1:A:48:ARG:NH2	7:A:601:HOH:O	2.37	0.44
4:C:504:FLC:HG1	5:C:505:NAD:C4N	2.48	0.44
1:C:132:ARG:HA	1:C:319:THR:O	2.18	0.43
1:A:37:GLU:HB3	1:A:67:ARG:HG2	2.00	0.43
1:A:427:LEU:O	1:A:428:ASP:HB2	2.18	0.43
1:B:244:PHE:O	1:B:248:MET:HG2	2.18	0.43
1:A:367:ILE:HG23	1:A:388:THR:HB	2.00	0.43
1:B:108:LEU:HB2	1:B:110:LEU:HD13	2.01	0.43
1:D:233:THR:O	1:D:276:LEU:HA	2.19	0.43
1:A:428:ASP:HA	7:A:809:HOH:O	2.18	0.42
1:C:97:THR:O	5:C:505:NAD:H2N	2.20	0.42
1:C:321:ASN:HB2	7:C:814:HOH:O	2.18	0.42
1:C:282:MET:HE2	1:D:306:ASP:O	2.19	0.42
1:A:129:THR:HG22	1:A:214:LEU:HG	2.02	0.42
1:D:261:VAL:HA	1:D:266:MET:O	2.20	0.42
1:D:148:VAL:HG11	1:D:308:LEU:HD11	2.02	0.41
1:B:128:ILE:HG22	1:B:129:THR:HG23	2.02	0.41
1:A:242:GLU:HB3	1:A:243:PRO:HD3	2.02	0.41
1:B:151:GLU:OE2	1:B:221:ARG:NE	2.48	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	403/418 (96%)	395 (98%)	7 (2%)	1 (0%)	47	37
1	B	403/418 (96%)	393 (98%)	9 (2%)	1 (0%)	47	37
1	C	403/418 (96%)	395 (98%)	7 (2%)	1 (0%)	47	37
1	D	403/418 (96%)	393 (98%)	9 (2%)	1 (0%)	47	37
All	All	1612/1672 (96%)	1576 (98%)	32 (2%)	4 (0%)	47	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	LYS
1	B	313	LYS
1	C	313	LYS
1	D	313	LYS

### 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	331/346 (96%)	329 (99%)	2 (1%)	86	86
1	B	327/346 (94%)	325 (99%)	2 (1%)	86	86
1	C	331/346 (96%)	329 (99%)	2 (1%)	86	86
1	D	330/346 (95%)	327 (99%)	3 (1%)	78	76
All	All	1319/1384 (95%)	1310 (99%)	9 (1%)	84	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASP
1	A	196	ASP
1	B	76	ASP
1	B	196	ASP
1	C	76	ASP
1	C	196	ASP
1	D	76	ASP
1	D	196	ASP
1	D	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	B	136	HIS
1	B	153	HIS
1	D	153	HIS
1	D	397	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	502	-	4,4,4	0.29	0	6,6,6	0.26	0
2	SO4	C	502	-	4,4,4	0.42	0	6,6,6	0.26	0
4	FLC	B	505	-	12,12,12	1.13	1 (8%)	17,17,17	1.38	2 (11%)
5	NAD	C	505	-	42,48,48	0.96	2 (4%)	50,73,73	1.42	7 (14%)
5	NAD	A	505	-	42,48,48	0.95	3 (7%)	50,73,73	1.30	6 (12%)
2	SO4	A	502	-	4,4,4	0.35	0	6,6,6	0.21	0
3	GOL	A	503	-	5,5,5	0.43	0	5,5,5	0.71	0
2	SO4	C	501	-	4,4,4	0.52	0	6,6,6	0.52	0
3	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.84	0
3	GOL	D	503	-	5,5,5	0.57	0	5,5,5	0.94	0
2	SO4	D	502	-	4,4,4	0.44	0	6,6,6	0.29	0
6	PEG	B	504	-	6,6,6	0.65	0	5,5,5	1.37	1 (20%)
2	SO4	D	501	-	4,4,4	0.65	0	6,6,6	0.27	0
4	FLC	D	505	-	12,12,12	2.29	5 (41%)	17,17,17	4.16	8 (47%)
2	SO4	A	501	-	4,4,4	0.49	0	6,6,6	0.40	0
3	GOL	C	503	-	5,5,5	0.32	0	5,5,5	0.24	0
4	FLC	A	504	-	12,12,12	1.13	1 (8%)	17,17,17	1.46	2 (11%)
5	NAD	D	506	-	42,48,48	1.03	2 (4%)	50,73,73	1.43	5 (10%)
4	FLC	C	504	-	12,12,12	1.25	1 (8%)	17,17,17	1.49	3 (17%)
2	SO4	B	501	-	4,4,4	0.46	0	6,6,6	0.26	0
3	GOL	D	504	-	5,5,5	0.29	0	5,5,5	0.29	0
5	NAD	B	506	-	42,48,48	0.97	2 (4%)	50,73,73	1.38	7 (14%)

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	GOL	D	503	-	-	0/4/4/4	-
5	NAD	C	505	-	-	3/26/62/62	0/5/5/5
5	NAD	A	505	-	-	4/26/62/62	0/5/5/5
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	D	504	-	-	2/4/4/4	-
6	PEG	B	504	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	D	506	-	-	3/26/62/62	0/5/5/5
4	FLC	C	504	-	-	7/16/16/16	-
4	FLC	D	505	-	-	6/16/16/16	-
4	FLC	A	504	-	-	5/16/16/16	-
3	GOL	C	503	-	-	2/4/4/4	-
5	NAD	B	506	-	-	3/26/62/62	0/5/5/5
3	GOL	B	503	-	-	0/4/4/4	-
4	FLC	B	505	-	-	7/16/16/16	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	505	FLC	CB-CBC	-5.60	1.47	1.53
5	D	506	NAD	PA-O3	3.80	1.63	1.59
5	B	506	NAD	PA-O3	3.42	1.63	1.59
4	D	505	FLC	CA-CB	-3.10	1.50	1.54
5	C	505	NAD	O4D-C1D	3.08	1.44	1.40
5	C	505	NAD	PA-O3	2.60	1.62	1.59
5	A	505	NAD	PA-O3	2.53	1.62	1.59
5	A	505	NAD	C2A-N3A	2.47	1.35	1.32
5	D	506	NAD	PN-O3	2.40	1.62	1.59
5	B	506	NAD	PN-O3	2.35	1.62	1.59
4	D	505	FLC	OHB-CB	2.31	1.47	1.43
4	A	504	FLC	OG2-CGC	-2.24	1.23	1.30
4	D	505	FLC	OG2-CGC	-2.24	1.23	1.30
4	C	504	FLC	CB-CBC	-2.17	1.51	1.53
4	B	505	FLC	CB-CBC	-2.09	1.51	1.53
4	D	505	FLC	OA2-CAC	-2.08	1.23	1.30
5	A	505	NAD	C3N-C7N	2.05	1.53	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	505	FLC	OHB-CB-CBC	-8.53	96.86	108.96
4	D	505	FLC	OHB-CB-CA	-7.62	91.99	109.38
4	D	505	FLC	OHB-CB-CG	-7.12	93.14	109.38
4	D	505	FLC	CB-CG-CGC	-6.61	95.84	113.92
5	C	505	NAD	N3A-C2A-N1A	-5.31	121.46	128.67
5	B	506	NAD	N3A-C2A-N1A	-4.85	122.09	128.67
5	D	506	NAD	N3A-C2A-N1A	-4.34	122.78	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	505	FLC	CA-CB-CBC	4.28	119.50	110.03
5	D	506	NAD	O7N-C7N-N7N	-4.27	116.45	122.62
4	D	505	FLC	CG-CB-CA	4.23	120.16	109.31
5	A	505	NAD	N3A-C2A-N1A	-4.01	123.22	128.67
4	D	505	FLC	CG-CB-CBC	4.01	118.90	110.03
5	A	505	NAD	O7N-C7N-N7N	-3.89	117.00	122.62
5	D	506	NAD	C3N-C7N-N7N	3.71	122.30	117.74
4	A	504	FLC	OB2-CBC-CB	3.63	120.11	113.14
5	C	505	NAD	O7N-C7N-N7N	-3.49	117.57	122.62
4	A	504	FLC	OB1-CBC-CB	-3.31	115.68	122.09
5	B	506	NAD	O3-PA-O1A	-3.19	101.11	110.70
5	B	506	NAD	O7N-C7N-N7N	-3.13	118.10	122.62
4	B	505	FLC	OG2-CGC-CG	3.10	124.18	114.35
5	C	505	NAD	C3N-C7N-N7N	3.00	121.43	117.74
4	C	504	FLC	OG2-CGC-CG	2.94	123.67	114.35
5	A	505	NAD	C3N-C7N-N7N	2.83	121.22	117.74
4	D	505	FLC	CB-CA-CAC	2.81	121.61	113.92
6	B	504	PEG	O2-C2-C1	2.72	122.09	110.11
5	C	505	NAD	O2A-PA-O3	-2.62	100.18	107.27
4	B	505	FLC	OG1-CGC-CG	-2.57	115.66	122.95
5	D	506	NAD	O3-PA-O1A	-2.38	103.54	110.70
5	B	506	NAD	C3N-C7N-N7N	2.32	120.60	117.74
5	A	505	NAD	O3-PN-O1N	-2.32	103.73	110.70
5	A	505	NAD	O2N-PN-O3	2.24	113.33	107.27
5	C	505	NAD	C2D-C3D-C4D	2.20	106.87	102.61
4	C	504	FLC	OG1-CGC-CG	-2.19	116.75	122.95
5	D	506	NAD	O3-PN-O1N	-2.19	104.12	110.70
5	C	505	NAD	N6A-C6A-N1A	2.15	122.93	118.33
5	A	505	NAD	N6A-C6A-N1A	2.15	122.92	118.33
5	C	505	NAD	C4B-O4B-C1B	2.08	111.83	109.92
4	C	504	FLC	OA2-CAC-CA	2.07	120.91	114.35
5	B	506	NAD	C4D-O4D-C1D	2.04	111.80	109.92
5	B	506	NAD	N6A-C6A-N1A	2.02	122.64	118.33
5	B	506	NAD	O2A-PA-O3	2.01	112.70	107.27

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	503	GOL	O2-C2-C3-O3
4	A	504	FLC	CG-CB-CBC-OB1
4	A	504	FLC	CG-CB-CBC-OB2
4	A	504	FLC	OHB-CB-CBC-OB1
4	A	504	FLC	OHB-CB-CBC-OB2
4	B	505	FLC	CG-CB-CBC-OB1
4	B	505	FLC	CG-CB-CBC-OB2
4	B	505	FLC	OHB-CB-CBC-OB1
4	B	505	FLC	OHB-CB-CBC-OB2
4	C	504	FLC	CG-CB-CBC-OB1
4	C	504	FLC	CG-CB-CBC-OB2
4	C	504	FLC	OHB-CB-CBC-OB1
4	C	504	FLC	OHB-CB-CBC-OB2
4	D	505	FLC	OHB-CB-CBC-OB1
4	D	505	FLC	OHB-CB-CBC-OB2
5	A	505	NAD	O4D-C1D-N1N-C2N
5	A	505	NAD	O4D-C1D-N1N-C6N
5	A	505	NAD	C2D-C1D-N1N-C2N
5	B	506	NAD	O4D-C1D-N1N-C2N
5	B	506	NAD	O4D-C1D-N1N-C6N
5	B	506	NAD	C2D-C1D-N1N-C2N
5	C	505	NAD	O4D-C1D-N1N-C2N
5	C	505	NAD	O4D-C1D-N1N-C6N
5	C	505	NAD	C2D-C1D-N1N-C2N
5	D	506	NAD	O4D-C1D-N1N-C2N
5	D	506	NAD	O4D-C1D-N1N-C6N
5	D	506	NAD	C2D-C1D-N1N-C2N
6	B	504	PEG	O2-C3-C4-O4
4	D	505	FLC	CA-CB-CG-CGC
3	D	504	GOL	O1-C1-C2-C3
3	D	504	GOL	O1-C1-C2-O2
3	A	503	GOL	O2-C2-C3-O3
4	A	504	FLC	CAC-CA-CB-OHB
4	C	504	FLC	CAC-CA-CB-OHB
4	D	505	FLC	OHB-CB-CG-CGC
3	A	503	GOL	C1-C2-C3-O3
4	B	505	FLC	CAC-CA-CB-OHB
4	C	504	FLC	CB-CG-CGC-OG2
4	C	504	FLC	CB-CG-CGC-OG1
5	A	505	NAD	C2D-C1D-N1N-C6N
6	B	504	PEG	O1-C1-C2-O2
4	D	505	FLC	CAC-CA-CB-CBC

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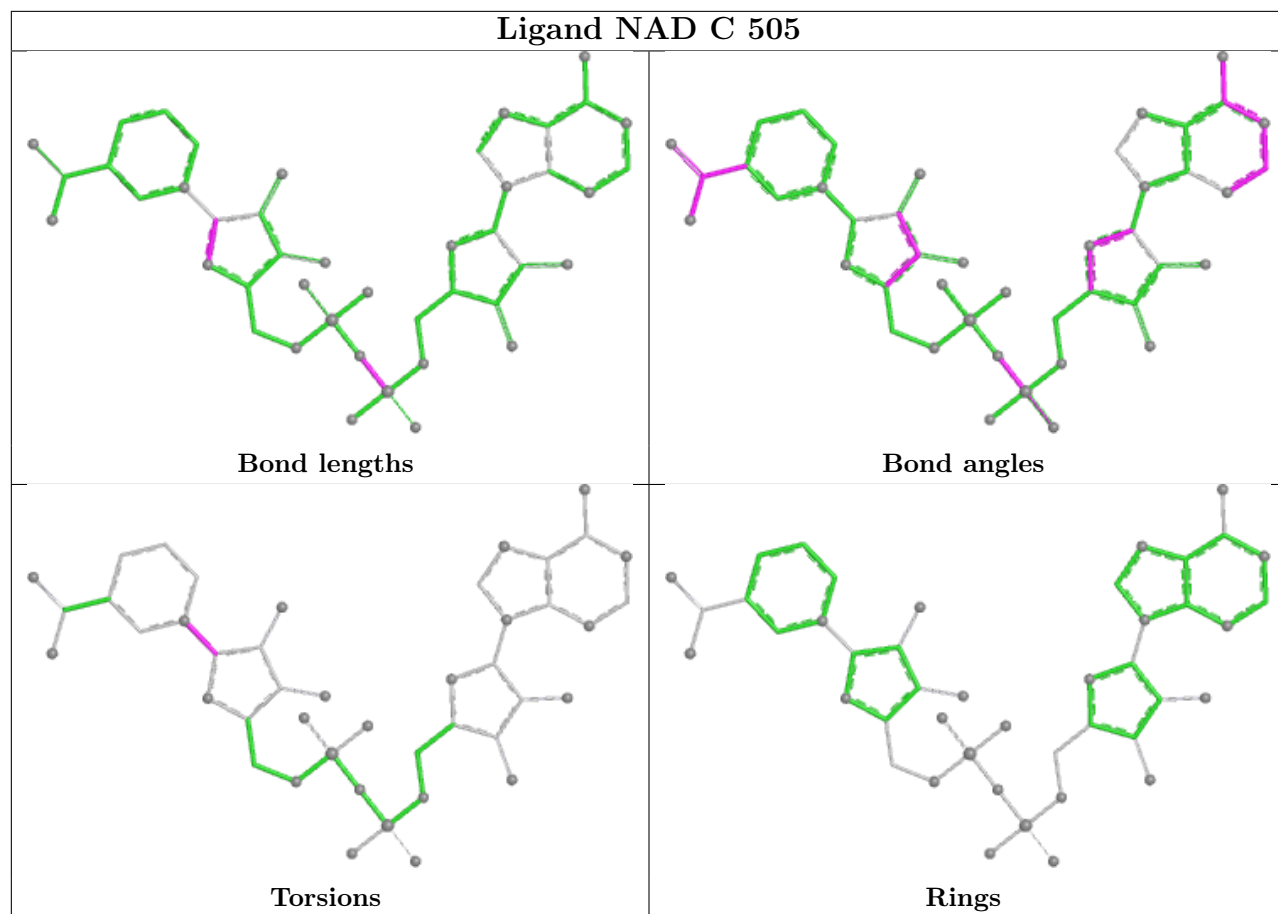
Mol	Chain	Res	Type	Atoms
4	D	505	FLC	CG-CB-CBC-OB1
4	B	505	FLC	CB-CG-CGC-OG2
4	B	505	FLC	CB-CG-CGC-OG1

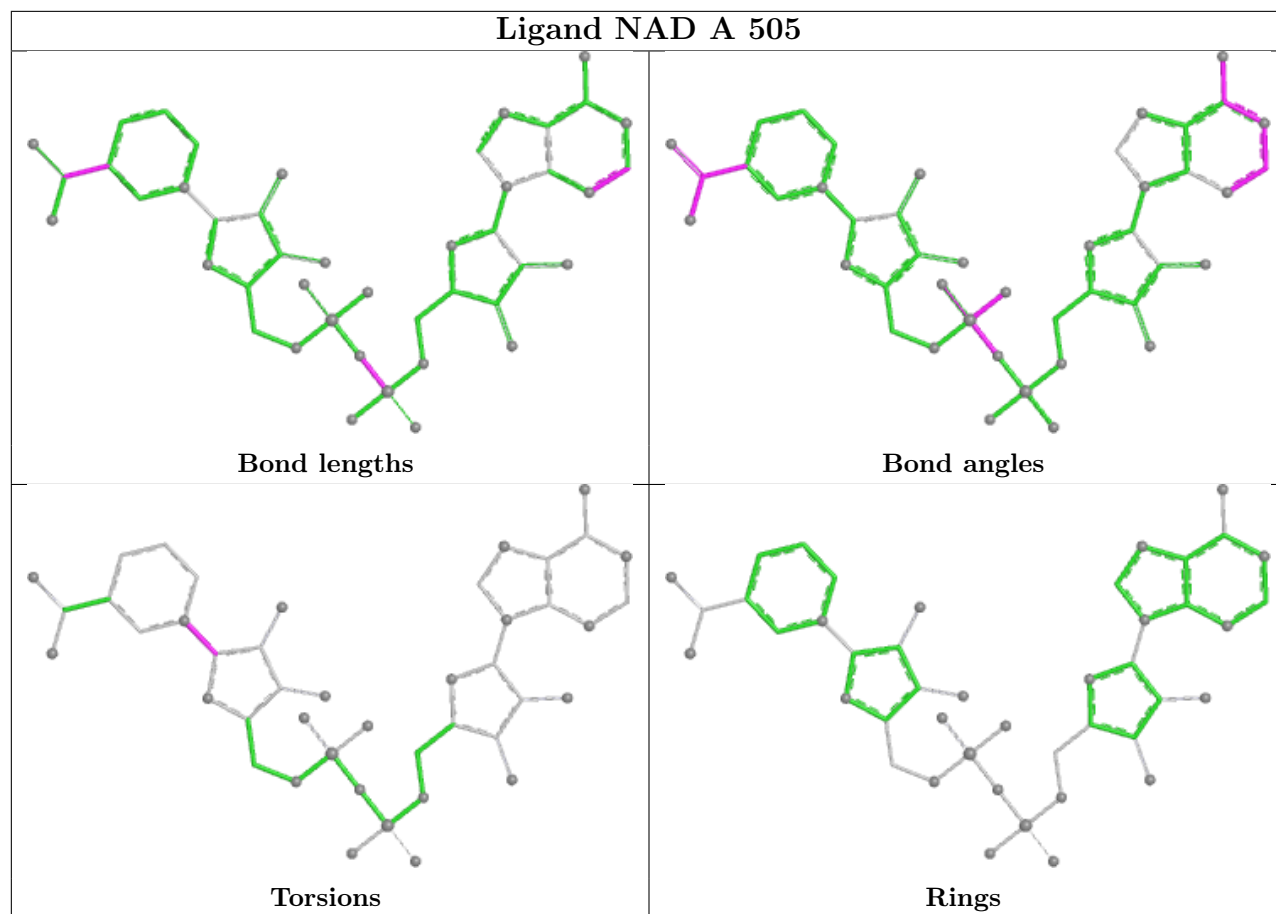
There are no ring outliers.

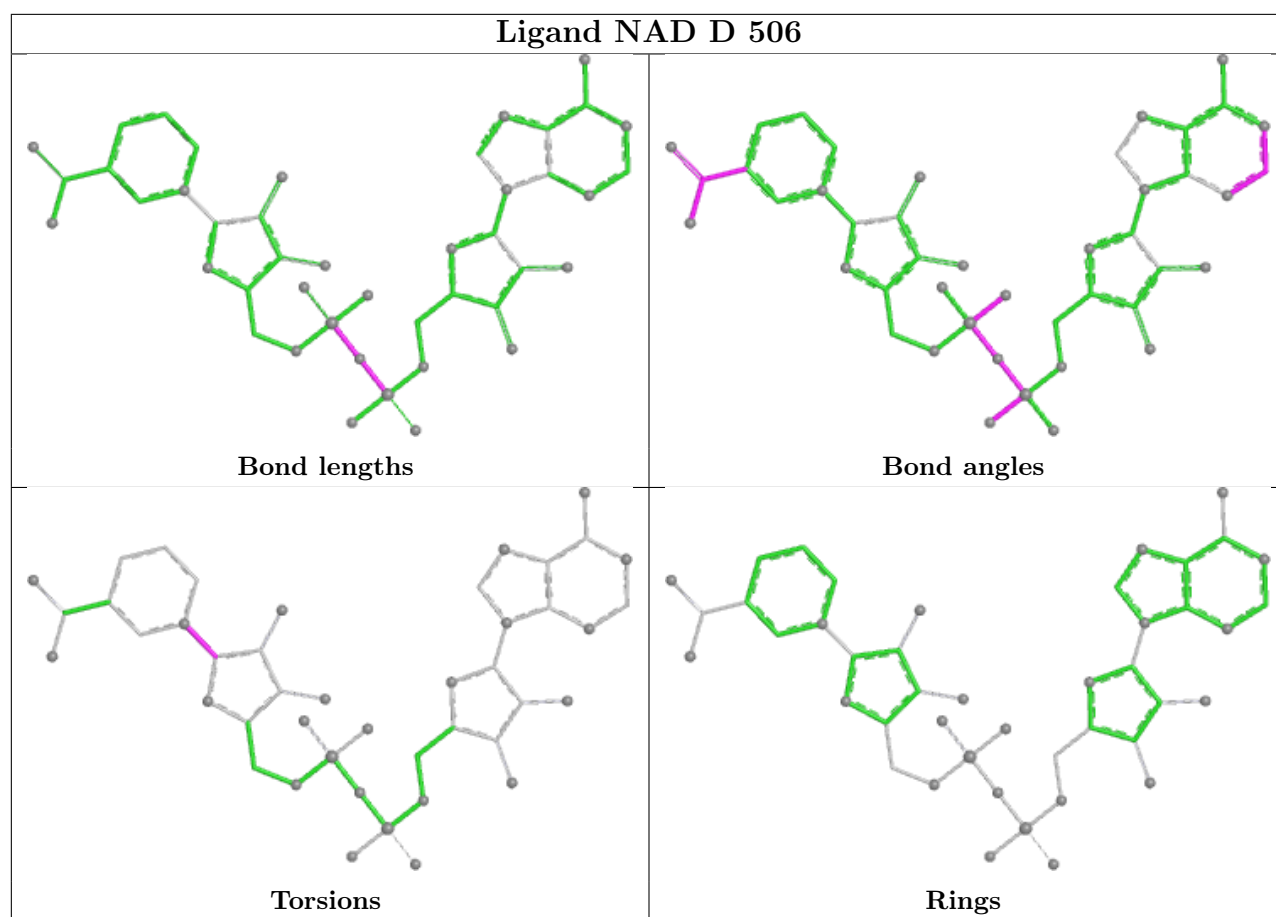
9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	FLC	1	0
5	C	505	NAD	2	0
5	A	505	NAD	2	0
3	B	503	GOL	1	0
6	B	504	PEG	10	0
4	D	505	FLC	1	0
5	D	506	NAD	2	0
4	C	504	FLC	1	0
5	B	506	NAD	2	0

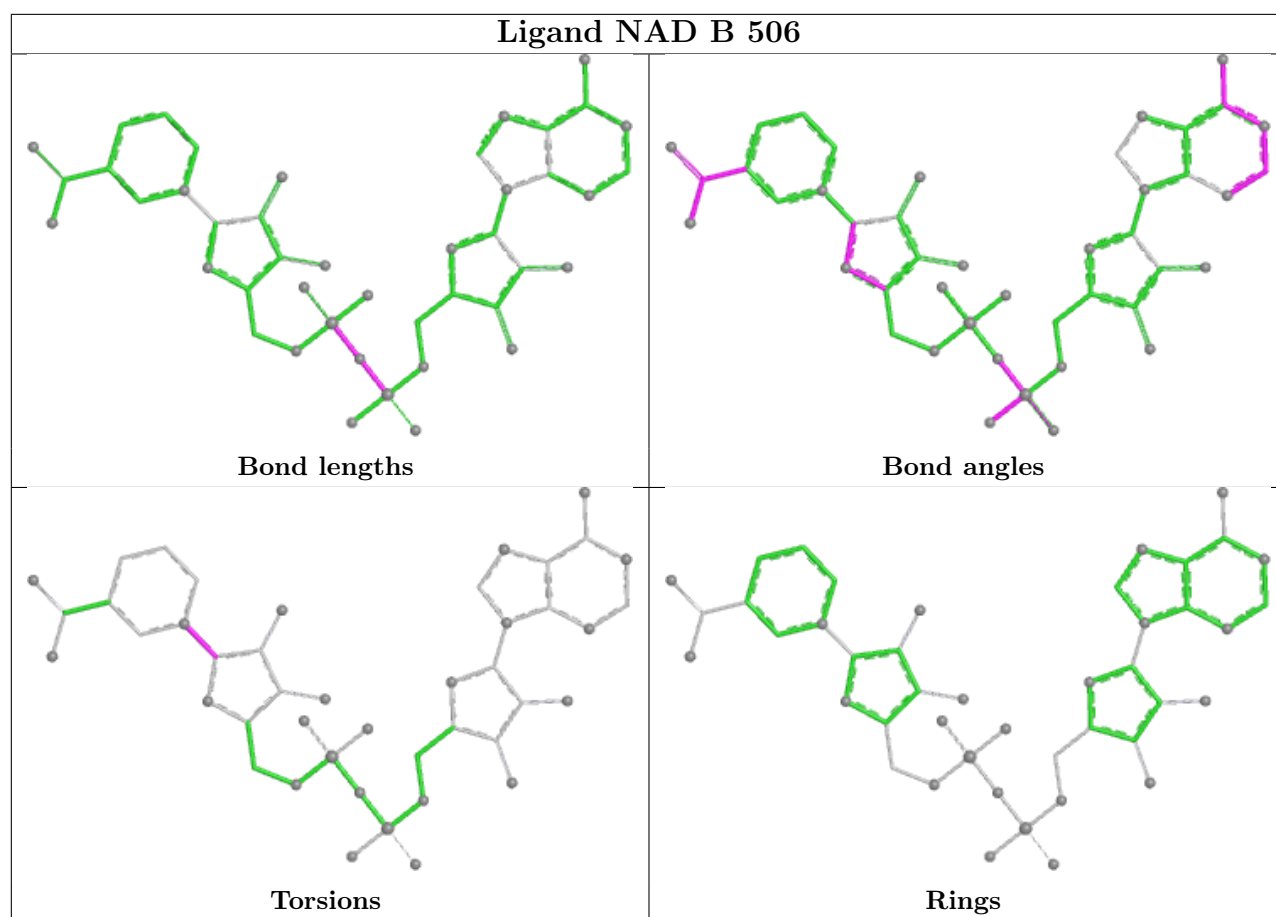
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	405/418 (96%)	-0.36	1 (0%) 95 95	5, 9, 24, 35	0
1	B	405/418 (96%)	-0.32	2 (0%) 91 91	5, 11, 25, 37	0
1	C	405/418 (96%)	-0.32	2 (0%) 91 91	4, 10, 26, 36	0
1	D	405/418 (96%)	-0.35	1 (0%) 95 95	5, 10, 24, 36	0
All	All	1620/1672 (96%)	-0.34	6 (0%) 92 93	4, 10, 25, 37	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ASP	3.7
1	A	428	ASP	2.8
1	C	428	ASP	2.8
1	C	181	PRO	2.7
1	D	181	PRO	2.7
1	B	108	LEU	2.6

### 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,

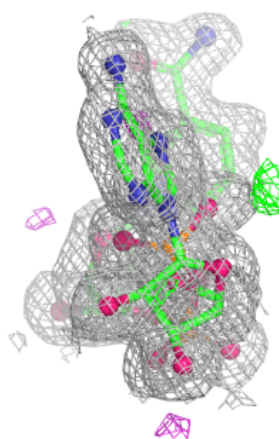
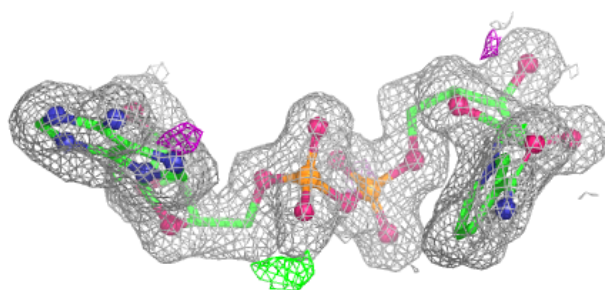
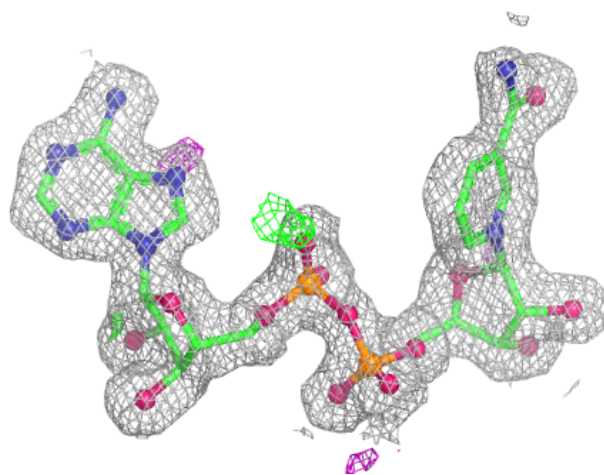
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	C	503	6/6	0.75	0.19	23,26,28,28	0
3	GOL	D	503	6/6	0.80	0.20	23,24,24,25	0
3	GOL	B	503	6/6	0.82	0.16	23,27,28,28	0
3	GOL	A	503	6/6	0.83	0.20	21,24,25,27	0
6	PEG	B	504	7/7	0.83	0.24	15,18,24,27	0
4	FLC	D	505	13/13	0.88	0.14	17,21,23,23	0
3	GOL	D	504	6/6	0.88	0.15	20,24,26,27	0
4	FLC	B	505	13/13	0.89	0.12	18,22,23,24	0
4	FLC	C	504	13/13	0.89	0.12	17,20,23,23	0
4	FLC	A	504	13/13	0.90	0.12	16,20,22,22	0
2	SO4	A	502	5/5	0.94	0.15	31,33,35,36	0
2	SO4	C	502	5/5	0.95	0.13	31,34,35,37	0
2	SO4	D	502	5/5	0.95	0.16	29,30,32,33	0
5	NAD	B	506	44/44	0.97	0.07	8,9,10,11	0
5	NAD	C	505	44/44	0.97	0.07	7,8,10,11	0
2	SO4	B	502	5/5	0.97	0.14	30,31,33,35	0
5	NAD	A	505	44/44	0.98	0.06	6,7,7,8	0
5	NAD	D	506	44/44	0.98	0.06	5,7,7,8	0
2	SO4	D	501	5/5	0.98	0.09	15,15,15,16	0
2	SO4	C	501	5/5	0.99	0.06	14,14,15,15	0
2	SO4	B	501	5/5	0.99	0.07	17,17,18,18	0
2	SO4	A	501	5/5	0.99	0.09	13,13,14,14	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.

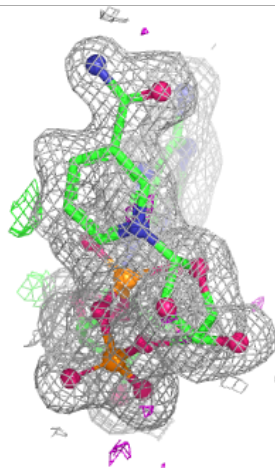
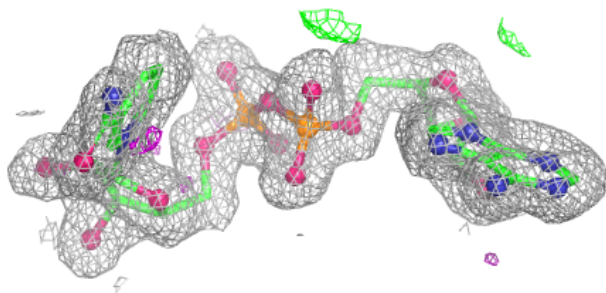
**Electron density around NAD B 506:**

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



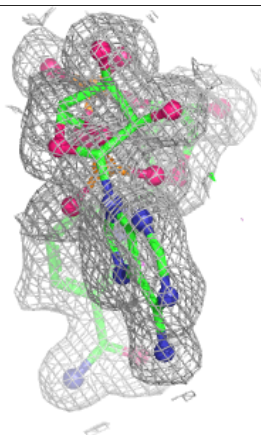
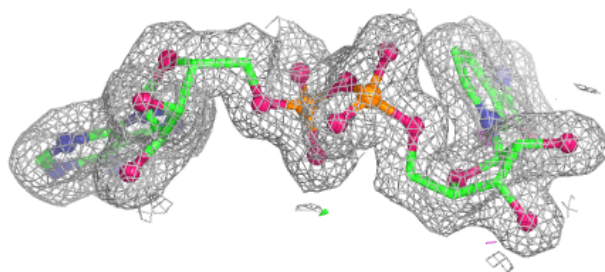
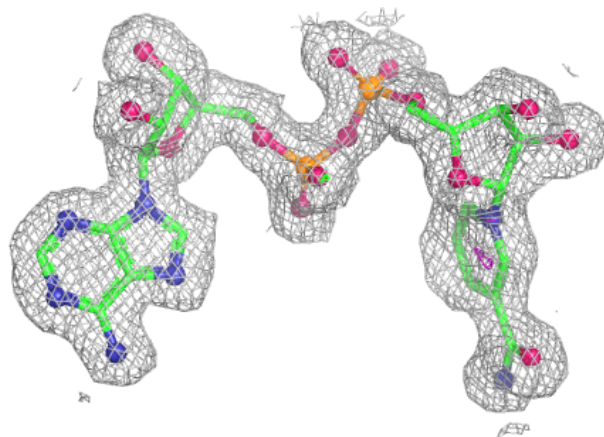
**Electron density around NAD C 505:**

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



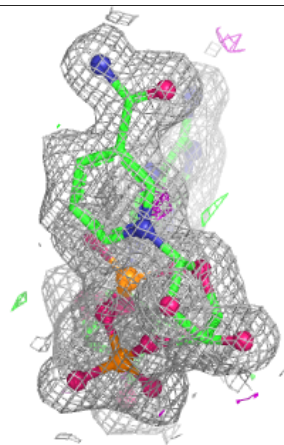
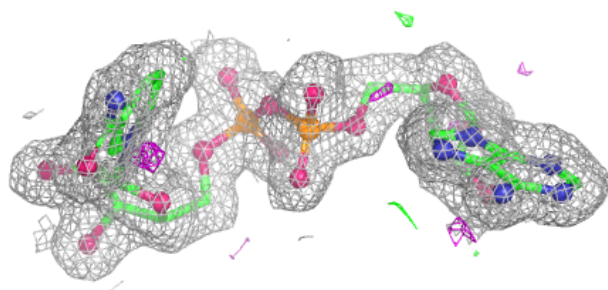
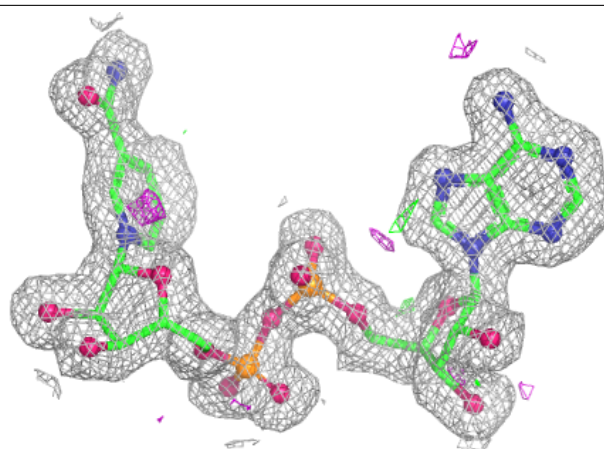
**Electron density around NAD A 505:**

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



**Electron density around NAD D 506:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.