



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:28 pm BST

PDB ID : 6UEK  
Title : Structure of Urocanate Hydratase from Trypanosoma cruzi in complex with NAD<sup>+</sup>  
Authors : Boreiko, S.; Silva, M.; Melo, R.F.P.; Silber, A.M.; Iulek, J.  
Deposited on : 2019-09-21  
Resolution : 2.16 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

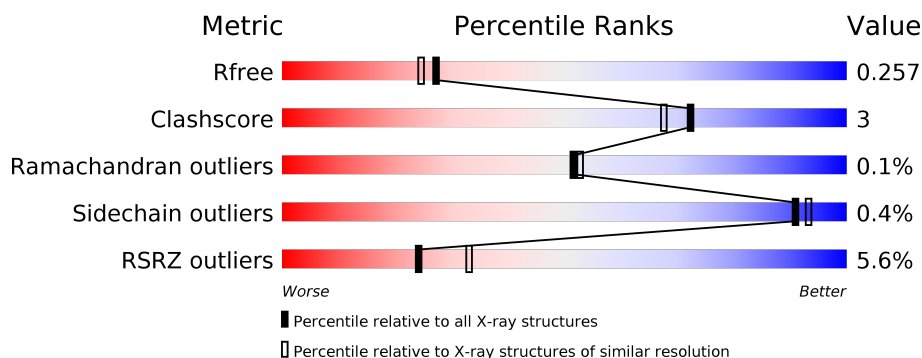
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	681	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 89%; height: 10px; background-color: green;"></div> <div style="width: 8%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> <div style="width: 100%; height: 10px; background-color: red;"></div> </div>
1	B	681	<div> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div>
1	C	681	<div> <div style="width: 6%; height: 10px; background-color: red;"></div> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div>
1	D	681	<div> <div style="width: 14%; height: 10px; background-color: red;"></div> <div style="width: 79%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19107 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 Urocanate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			4975	3142	874	923	36			
1	B	654	Total	C	N	O	S	0	4	2
			4926	3106	858	926	36			
1	C	641	Total	C	N	O	S	0	0	1
			4531	2846	791	862	32			
1	D	588	Total	C	N	O	S	0	0	3
			3917	2427	710	751	29			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	676	HIS	-	expression tag	UNP Q4D9S6
A	677	HIS	-	expression tag	UNP Q4D9S6
A	678	HIS	-	expression tag	UNP Q4D9S6
A	679	HIS	-	expression tag	UNP Q4D9S6
A	680	HIS	-	expression tag	UNP Q4D9S6
A	681	HIS	-	expression tag	UNP Q4D9S6
B	676	HIS	-	expression tag	UNP Q4D9S6
B	677	HIS	-	expression tag	UNP Q4D9S6
B	678	HIS	-	expression tag	UNP Q4D9S6
B	679	HIS	-	expression tag	UNP Q4D9S6
B	680	HIS	-	expression tag	UNP Q4D9S6
B	681	HIS	-	expression tag	UNP Q4D9S6
C	676	HIS	-	expression tag	UNP Q4D9S6
C	677	HIS	-	expression tag	UNP Q4D9S6
C	678	HIS	-	expression tag	UNP Q4D9S6
C	679	HIS	-	expression tag	UNP Q4D9S6
C	680	HIS	-	expression tag	UNP Q4D9S6
C	681	HIS	-	expression tag	UNP Q4D9S6
D	676	HIS	-	expression tag	UNP Q4D9S6
D	677	HIS	-	expression tag	UNP Q4D9S6
D	678	HIS	-	expression tag	UNP Q4D9S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	679	HIS	-	expression tag	UNP Q4D9S6
D	680	HIS	-	expression tag	UNP Q4D9S6
D	681	HIS	-	expression tag	UNP Q4D9S6

- # NAD

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	231	Total O 231 231	0	0
3	B	210	Total O 210 210	0	0
3	C	81	Total O 81 81	0	0



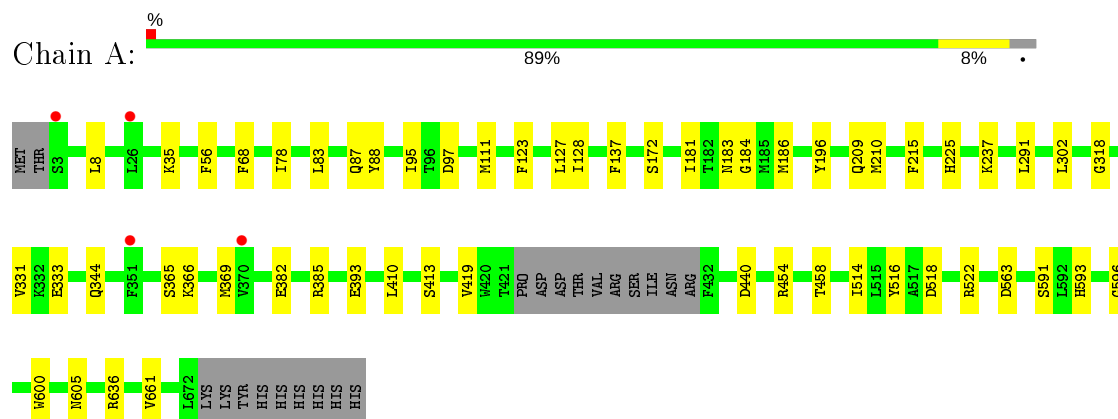
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	60	Total	O	0	0
			60	60		

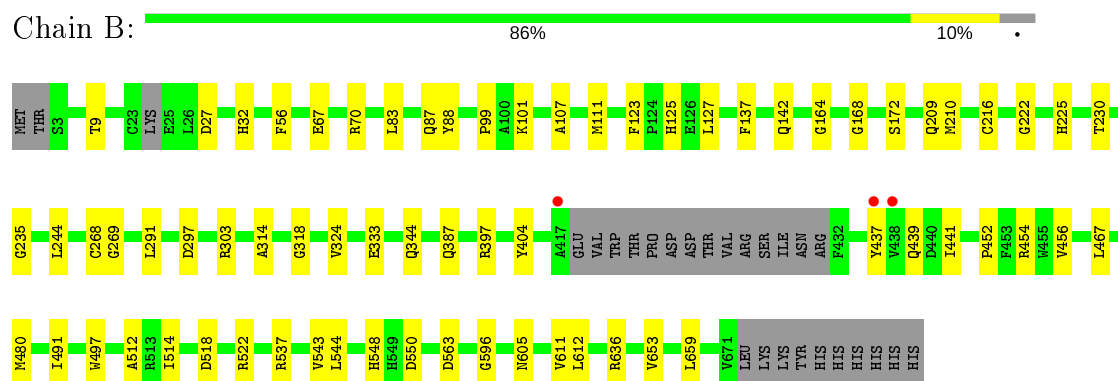
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

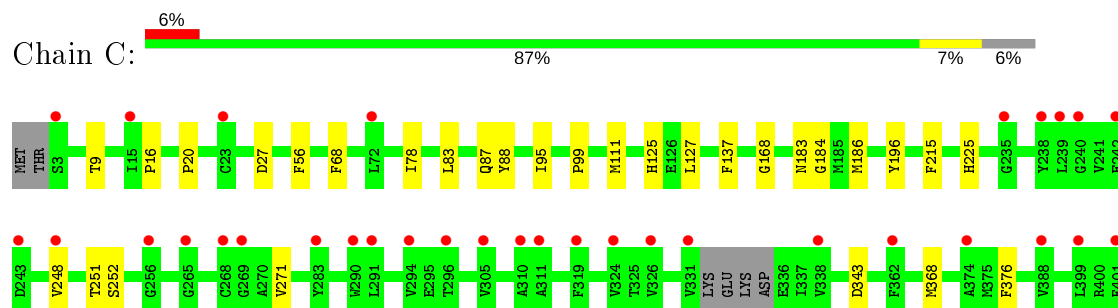
#### • Molecule 1: Urocanate hydratase

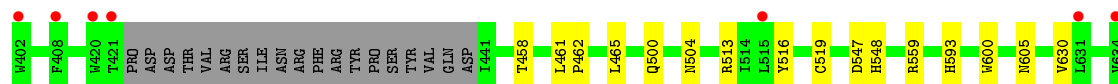


#### • Molecule 1: Urocanate hydratase

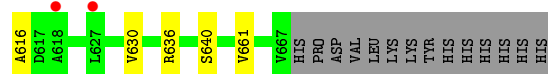
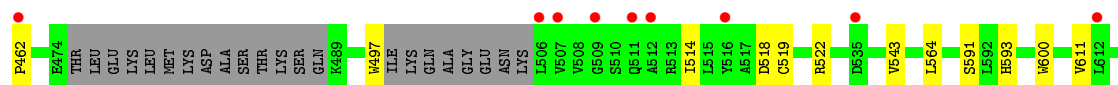
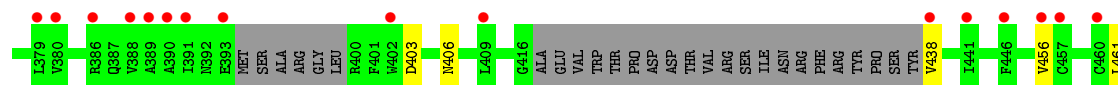
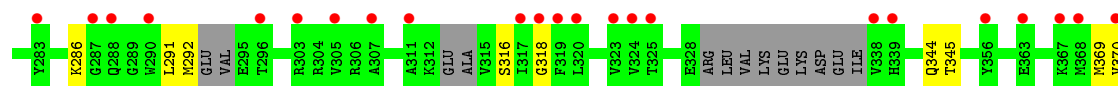
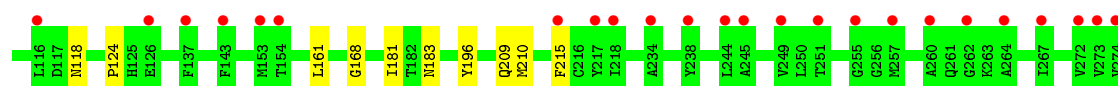
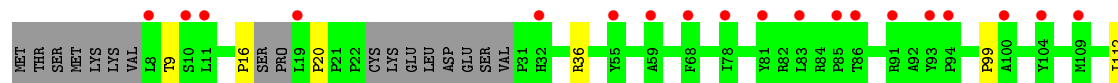
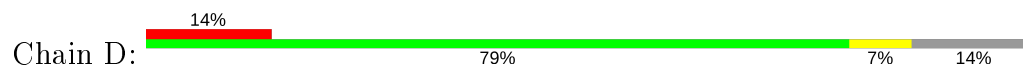


#### • Molecule 1: Urocanate hydratase





● Molecule 1: Urocanate hydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.61Å 134.79Å 113.40Å 90.00° 93.25° 90.00°	Depositor
Resolution (Å)	113.22 – 2.16 30.01 – 2.16	Depositor EDS
% Data completeness (in resolution range)	94.3 (113.22-2.16) 94.4 (30.01-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.218 , 0.255 0.227 , 0.257	Depositor DCC
$R_{free}$ test set	1886 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19107	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: NAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.21	0/5088	0.38	0/6915
1	B	0.21	0/5057	0.37	0/6876
1	C	0.20	0/4630	0.36	0/6328
1	D	0.20	0/3989	0.36	0/5458
All	All	0.20	0/18764	0.37	0/25577

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4975	0	4731	30	0
1	B	4926	0	4679	39	0
1	C	4531	0	4021	26	0
1	D	3917	0	3244	28	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
2	C	44	0	7	0	0
2	D	44	0	7	1	0
3	A	231	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	210	0	0	3	0
3	C	81	0	0	0	0
3	D	60	0	0	1	0
All	All	19107	0	16741	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (119) 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:344:GLN:NE2	2:A:701:NAD:O7N	2.23	0.71
1:B:101:LYS:HB3	1:D:616:ALA:HB2	1.74	0.69
1:C:500:GLN:O	1:C:504:ASN:ND2	2.27	0.68
1:A:127:LEU:HD22	1:A:137:PHE:HB2	1.76	0.67
1:C:127:LEU:HD22	1:C:137:PHE:HB2	1.77	0.67
1:D:543:VAL:HG22	1:D:611:VAL:HG22	1.77	0.67
1:D:497:TRP:NE1	1:D:514:ILE:O	2.31	0.62
1:D:292:MET:N	1:D:316:SER:OG	2.33	0.62
1:B:344:GLN:NE2	2:B:701:NAD:O7N	2.34	0.60
1:B:67:GLU:HG3	1:B:70:ARG:HH21	1.67	0.60
1:B:303:ARG:NH2	3:B:805:HOH:O	2.30	0.59
1:D:16:PRO:HG2	1:D:20:PRO:HD3	1.84	0.59
1:A:291:LEU:HD21	1:A:318:GLY:HA3	1.84	0.59
1:B:127:LEU:HD22	1:B:137:PHE:HB2	1.85	0.59
1:D:344:GLN:NE2	2:D:701[A]:NAD:O7N	2.36	0.59
1:A:237:LYS:NZ	1:A:440:ASP:O	2.36	0.58
1:A:35:LYS:NZ	3:A:807:HOH:O	2.36	0.57
1:D:456:VAL:HG22	1:D:543:VAL:HB	1.87	0.57
1:B:291:LEU:HD21	1:B:318:GLY:HA3	1.87	0.56
1:C:661:VAL:HA	1:D:168:GLY:HA3	1.88	0.55
1:A:123:PHE:HB2	1:A:128:ILE:HB	1.89	0.54
1:B:397:ARG:NH1	3:B:811:HOH:O	2.40	0.54
1:D:291:LEU:HD21	1:D:318:GLY:HA3	1.90	0.54
1:D:9:THR:HA	1:D:99:PRO:HG3	1.90	0.54
1:C:16:PRO:HG2	1:C:20:PRO:HD3	1.89	0.53
1:D:286:LYS:HA	1:D:291:LEU:HB3	1.90	0.53
1:D:118:ASN:HA	1:D:124:PRO:HG3	1.90	0.53
1:C:95:ILE:HB	1:C:458:THR:HB	1.90	0.52
1:C:248:VAL:HG22	1:C:271:VAL:HB	1.91	0.52
1:B:543:VAL:HG22	1:B:611:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ASP:OD2	3:B:801:HOH:O	2.19	0.51
1:D:369:MET:HG3	1:D:370:VAL:HG13	1.91	0.51
1:C:183:ASN:HB2	1:C:593:HIS:CD2	2.45	0.51
1:C:547:ASP:OD1	1:C:548:HIS:N	2.44	0.50
1:A:344:GLN:HG2	2:A:701:NAD:H51N	1.92	0.50
1:A:331:VAL:HG13	1:A:393:GLU:HG2	1.95	0.48
1:A:68:PHE:HB3	1:A:78:ILE:HD13	1.95	0.48
1:A:183:ASN:HB2	1:A:593:HIS:CD2	2.48	0.48
1:B:456:VAL:HG22	1:B:512:ALA:HB2	1.95	0.48
1:B:439:GLN:HA	1:B:563:ASP:HB3	1.95	0.48
1:C:27:ASP:HB3	1:C:125:HIS:HE1	1.77	0.48
1:B:235:GLY:HA3	1:B:244:LEU:HD21	1.96	0.47
1:B:230:THR:HG23	1:B:441:ILE:HD11	1.96	0.47
1:B:467:LEU:HD21	1:B:537:ARG:HB3	1.97	0.47
1:B:333:GLU:O	1:B:397:ARG:NH2	2.47	0.47
1:B:222:GLY:HA2	1:B:514:ILE:HG21	1.97	0.46
1:C:184:GLY:O	1:C:186:MET:HG2	2.15	0.46
1:A:95:ILE:HB	1:A:458:THR:HB	1.97	0.46
1:B:216:CYS:O	1:B:454:ARG:NH1	2.46	0.46
1:A:410:LEU:O	1:A:413:SER:OG	2.24	0.46
1:D:196:TYR:HB2	1:D:600:TRP:CE2	2.51	0.46
1:C:368:MET:HG2	1:C:376:PHE:HB2	1.98	0.46
1:B:9:THR:HA	1:B:99:PRO:HG3	1.98	0.45
1:C:225:HIS:CE1	1:C:516:TYR:H	2.35	0.45
1:C:196:TYR:HB2	1:C:600:TRP:CE2	2.51	0.45
1:C:251:THR:OG1	1:C:252:SER:N	2.50	0.45
1:A:413:SER:HB3	1:A:419:VAL:HG21	1.99	0.45
1:D:209:GLN:HB3	1:D:210:MET:H	1.57	0.44
1:A:184:GLY:O	1:A:186:MET:HG2	2.17	0.44
1:B:210:MET:SD	1:B:548:HIS:HB2	2.57	0.44
1:B:244:LEU:HD12	1:B:268:CYS:HB3	2.00	0.44
1:B:87:GLN:HG2	1:B:88:TYR:HD2	1.82	0.44
1:A:8:LEU:HD12	1:A:97:ASP:HB3	1.98	0.44
1:B:209:GLN:HB3	1:B:210:MET:H	1.48	0.44
1:A:366:LYS:HA	1:A:369:MET:HE3	2.00	0.44
1:D:403:ASP:O	1:D:438:VAL:N	2.51	0.44
1:C:9:THR:HA	1:C:99:PRO:HG3	2.00	0.44
1:D:181:ILE:O	1:D:591:SER:HA	2.17	0.44
1:C:168:GLY:HA3	1:D:661:VAL:HA	1.99	0.44
1:C:465:LEU:HD11	1:C:513:ARG:HB2	2.00	0.43
1:A:382:GLU:HG2	1:A:385:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:TYR:HB2	1:A:600:TRP:CE2	2.53	0.43
1:A:596:GLY:HA3	1:A:605:ASN:ND2	2.33	0.43
1:B:27:ASP:O	1:B:32:HIS:NE2	2.33	0.43
1:A:225:HIS:HE1	1:A:516:TYR:CD1	2.37	0.43
1:A:661:VAL:HA	1:B:168:GLY:HA3	1.99	0.43
1:B:225:HIS:HB2	1:B:497:TRP:CZ2	2.54	0.43
1:C:111:MET:HB3	1:C:215:PHE:O	2.18	0.43
1:C:252:SER:OG	1:C:343:ASP:OD1	2.35	0.43
1:C:461:LEU:HA	1:C:462:PRO:HD3	1.92	0.43
1:B:107:ALA:O	1:B:111:MET:HG2	2.19	0.43
1:B:653:VAL:HA	1:B:659:LEU:HD23	2.01	0.43
1:B:452:PRO:HD2	1:B:550:ASP:OD1	2.18	0.42
1:D:112:ILE:HG12	1:D:215:PHE:CG	2.54	0.42
1:A:302:LEU:HD13	1:A:333:GLU:HG3	2.01	0.42
1:B:480:MET:HB2	1:B:491:ILE:HG21	2.02	0.42
1:D:36:ARG:NH1	3:D:805:HOH:O	2.43	0.42
1:A:209:GLN:HB3	1:A:210:MET:H	1.54	0.42
1:A:518:ASP:O	1:A:522:ARG:HG3	2.19	0.42
1:A:87:GLN:HG2	1:A:88:TYR:HD2	1.84	0.42
1:C:87:GLN:HG3	1:C:88:TYR:CD2	2.54	0.42
1:A:111:MET:HB3	1:A:215:PHE:O	2.19	0.42
1:C:519:CYS:HB2	1:C:630:VAL:HG11	2.01	0.42
1:C:27:ASP:HB3	1:C:125:HIS:CE1	2.53	0.42
1:B:56:PHE:CE2	1:B:83:LEU:HD11	2.55	0.42
1:B:544:LEU:HD11	1:B:612:LEU:HD11	2.02	0.42
1:C:56:PHE:CE2	1:C:83:LEU:HD11	2.54	0.42
1:C:68:PHE:HB3	1:C:78:ILE:HD13	2.02	0.42
1:D:518:ASP:O	1:D:522:ARG:HG3	2.19	0.42
1:B:518:ASP:O	1:B:522:ARG:HG3	2.19	0.41
1:B:142:GLN:HB3	1:B:164:GLY:O	2.21	0.41
1:B:596:GLY:HA3	1:B:605:ASN:ND2	2.36	0.41
1:B:27:ASP:HB3	1:B:125:HIS:CE1	2.55	0.41
1:A:181:ILE:O	1:A:591:SER:HA	2.20	0.41
1:C:593:HIS:HB2	1:C:605:ASN:ND2	2.35	0.41
1:D:345:THR:O	1:D:406:ASN:ND2	2.48	0.41
1:D:519:CYS:HB2	1:D:630:VAL:HG11	2.03	0.41
1:B:269:GLY:HA2	1:B:314:ALA:HB2	2.03	0.41
1:D:183:ASN:HB2	1:D:593:HIS:CD2	2.55	0.41
1:B:297:ASP:OD1	1:B:297:ASP:N	2.48	0.41
1:D:161:LEU:HD12	1:D:181:ILE:HG12	2.01	0.41
1:D:564:LEU:HD22	1:D:640:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:LEU:HA	1:D:462:PRO:HD2	1.86	0.40
1:A:365:SER:O	1:A:369:MET:HB2	2.21	0.40
1:A:454:ARG:HH21	1:A:514:ILE:HD12	1.86	0.40
1:A:56:PHE:CE1	1:A:83:LEU:HD11	2.56	0.40
1:B:324:VAL:HG22	1:B:387:GLN:HB2	2.04	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	656/681 (96%)	635 (97%)	20 (3%)	1 (0%)	47	46
1	B	652/681 (96%)	630 (97%)	21 (3%)	1 (0%)	47	46
1	C	635/681 (93%)	615 (97%)	19 (3%)	1 (0%)	47	46
1	D	568/681 (83%)	544 (96%)	24 (4%)	0	100	100
All	All	2511/2724 (92%)	2424 (96%)	84 (3%)	3 (0%)	51	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	C	559	ARG
1	B	172	SER

### 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	493/562 (88%)	491 (100%)	2 (0%)	91	93
1	B	496/562 (88%)	493 (99%)	3 (1%)	86	90
1	C	405/562 (72%)	404 (100%)	1 (0%)	93	96
1	D	308/562 (55%)	307 (100%)	1 (0%)	92	95
All	All	1702/2248 (76%)	1695 (100%)	7 (0%)	91	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	ASP
1	A	636	ARG
1	B	404	TYR
1	B	437	TYR
1	B	636	ARG
1	C	636	ARG
1	D	636	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	HIS
1	C	125	HIS
1	C	523	GLN
1	C	646	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	B	701	-	42,48,48	0.55	0	50,73,73	0.62	1 (2%)
2	NAD	A	701	-	42,48,48	0.55	0	50,73,73	0.62	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	701	-	-	1/26/62/62	0/5/5/5
2	NAD	A	701	-	-	6/26/62/62	0/5/5/5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	NAD	C5A-C6A-N6A	2.31	123.86	120.35
2	A	701	NAD	C5A-C6A-N6A	2.31	123.86	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NAD	C5B-O5B-PA-O1A
2	A	701	NAD	PN-O3-PA-O5B
2	A	701	NAD	O4B-C4B-C5B-O5B
2	A	701	NAD	C5B-O5B-PA-O3
2	A	701	NAD	C5B-O5B-PA-O2A
2	B	701	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	701	NAD	C3B-C4B-C5B-O5B

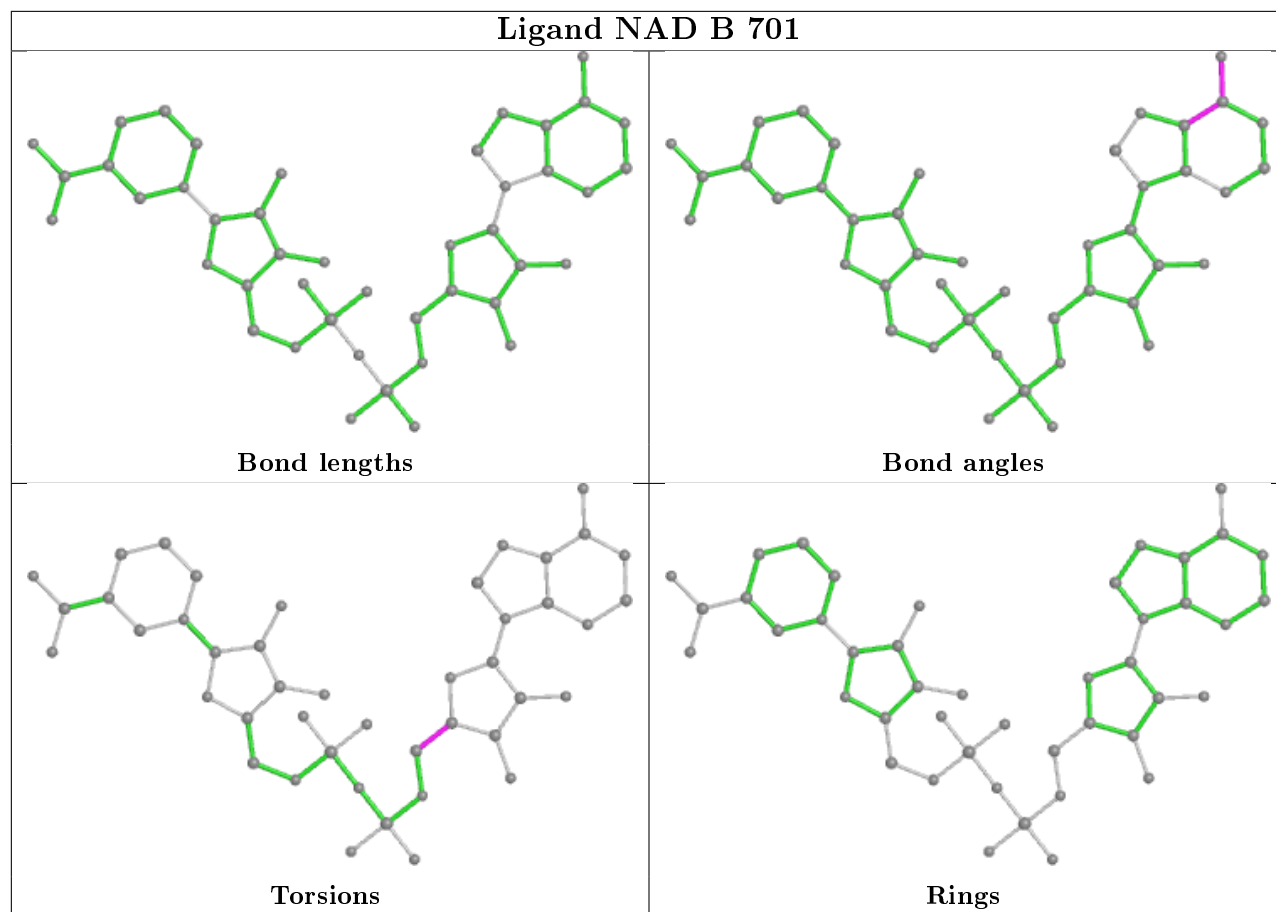
There are no ring outliers.

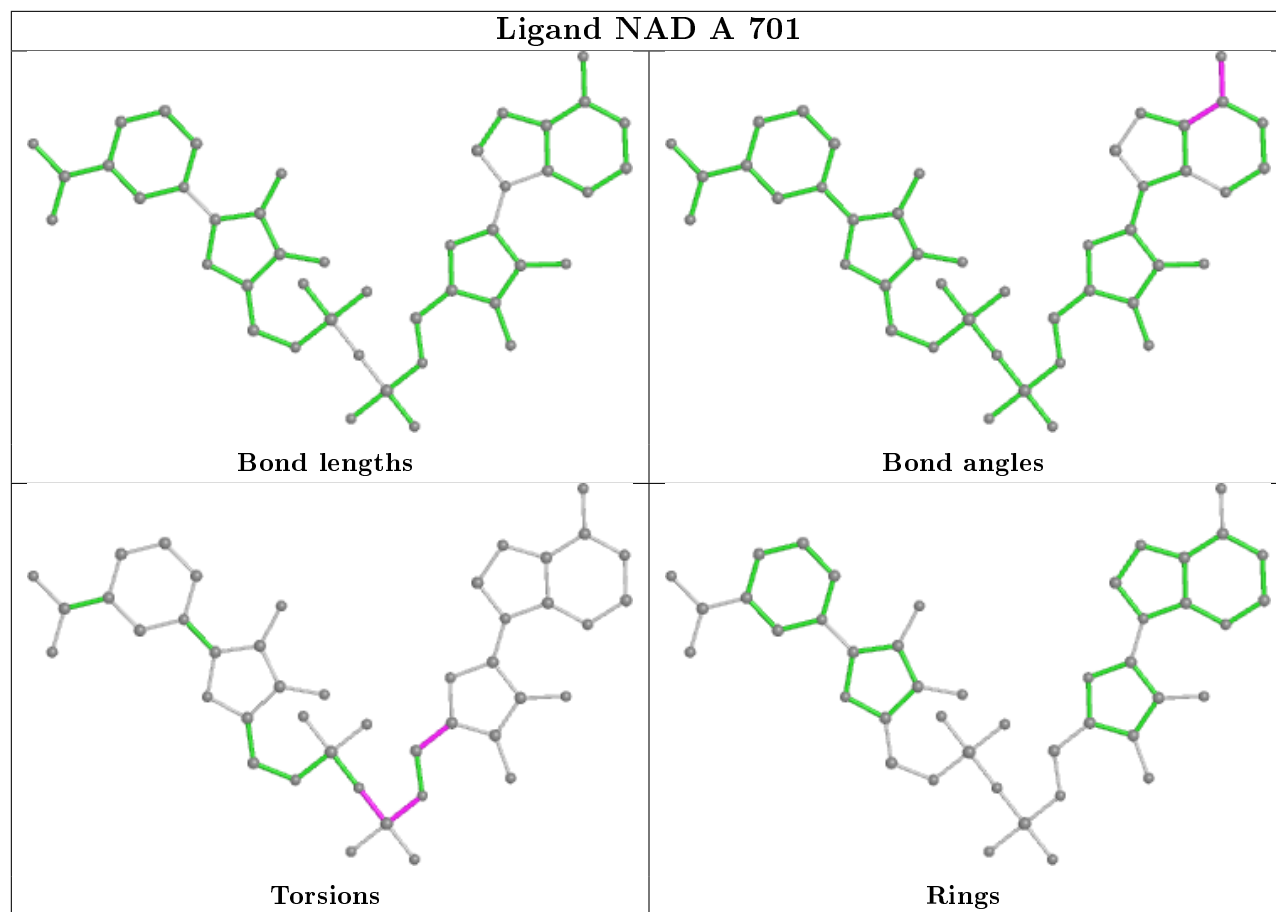
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	NAD	1	0
2	A	701	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	660/681 (96%)	0.05	4 (0%) 89 91	25, 38, 63, 99	0
1	B	654/681 (96%)	0.02	3 (0%) 91 93	24, 39, 60, 89	0
1	C	641/681 (94%)	0.46	43 (6%) 17 24	32, 56, 93, 148	0
1	D	588/681 (86%)	0.93	93 (15%) 2 2	30, 74, 116, 163	0
All	All	2543/2724 (93%)	0.35	143 (5%) 24 33	24, 47, 95, 163	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	ALA	14.3
1	D	238	TYR	7.1
1	D	305	VAL	7.1
1	C	291	LEU	6.6
1	D	68	PHE	5.9
1	C	239	LEU	5.8
1	C	420	TRP	5.8
1	D	320	LEU	5.5
1	D	386	ARG	5.5
1	C	310	ALA	5.5
1	C	240	GLY	5.1
1	D	391	ILE	5.0
1	D	338	VAL	4.9
1	C	238	TYR	4.7
1	D	441	ILE	4.5
1	D	390	ALA	4.3
1	D	296	THR	4.3
1	D	318	GLY	4.3
1	D	94	PRO	4.0
1	C	242	GLU	4.0
1	D	100	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	272	VAL	3.9
1	D	457	CYS	3.9
1	C	296	THR	3.9
1	C	388	VAL	3.8
1	D	307	ALA	3.8
1	D	274	VAL	3.7
1	C	243	ASP	3.7
1	D	283	TYR	3.6
1	D	460	CYS	3.6
1	D	317	ILE	3.6
1	C	326	VAL	3.5
1	D	290	TRP	3.5
1	D	217	TYR	3.5
1	D	154	THR	3.4
1	D	143	PHE	3.4
1	D	83	LEU	3.4
1	C	421	THR	3.4
1	C	256	GLY	3.4
1	D	244	LEU	3.3
1	D	368	MET	3.3
1	D	59	ALA	3.2
1	C	515	LEU	3.2
1	D	104	TYR	3.2
1	D	85	PRO	3.1
1	D	324	VAL	3.1
1	D	153	MET	3.1
1	D	456	VAL	3.1
1	A	26	LEU	3.1
1	D	86	THR	3.0
1	D	380	VAL	2.9
1	C	319	PHE	2.9
1	D	267	ILE	2.9
1	D	402	TRP	2.9
1	D	234	ALA	2.9
1	C	399	LEU	2.9
1	A	3	SER	2.9
1	D	511	GLN	2.8
1	D	363	GLU	2.8
1	D	409	LEU	2.8
1	C	235	GLY	2.8
1	C	3	SER	2.8
1	C	269	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	507	VAL	2.8
1	C	362	PHE	2.8
1	D	257	MET	2.8
1	D	264	ALA	2.8
1	C	408	PHE	2.7
1	D	116	LEU	2.7
1	C	290	TRP	2.7
1	D	627	LEU	2.7
1	D	255	GLY	2.7
1	C	248	VAL	2.7
1	C	338	VAL	2.7
1	D	509	GLY	2.7
1	D	612	LEU	2.7
1	D	379	LEU	2.6
1	C	305	VAL	2.6
1	D	356	TYR	2.6
1	D	388	VAL	2.6
1	D	339	HIS	2.6
1	D	393	GLU	2.6
1	C	311	ALA	2.6
1	D	10	SER	2.5
1	D	323	VAL	2.5
1	C	374	ALA	2.5
1	D	273	VAL	2.5
1	D	251	THR	2.5
1	C	324	VAL	2.5
1	D	81	TYR	2.5
1	A	351	PHE	2.5
1	C	664	PRO	2.4
1	D	325	THR	2.4
1	A	370	VAL	2.4
1	C	634	VAL	2.4
1	D	32	HIS	2.4
1	D	109	MET	2.4
1	D	78	ILE	2.4
1	D	506	LEU	2.3
1	C	643	ALA	2.3
1	D	618	ALA	2.3
1	D	91	ARG	2.3
1	D	137	PHE	2.3
1	B	417	ALA	2.3
1	D	367	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	218	ILE	2.3
1	D	389	ALA	2.3
1	D	249	VAL	2.3
1	B	437	TYR	2.2
1	D	19	LEU	2.2
1	D	288	GLN	2.2
1	D	319	PHE	2.2
1	D	462	PRO	2.2
1	C	657	GLU	2.2
1	C	72	LEU	2.2
1	C	401	PHE	2.2
1	D	93	TYR	2.2
1	D	512	ALA	2.2
1	C	331	VAL	2.1
1	D	215	PHE	2.1
1	D	446	PHE	2.1
1	C	23	CYS	2.1
1	D	8	LEU	2.1
1	C	265	GLY	2.1
1	C	283	TYR	2.1
1	C	631	LEU	2.1
1	D	287	GLY	2.1
1	B	438	VAL	2.1
1	D	535	ASP	2.1
1	D	311	ALA	2.1
1	C	402	TRP	2.1
1	D	126	GLU	2.0
1	C	15	ILE	2.0
1	D	370	VAL	2.0
1	D	55	TYR	2.0
1	D	262	GLY	2.0
1	D	516	TYR	2.0
1	D	260	ALA	2.0
1	C	294	VAL	2.0
1	D	11	LEU	2.0
1	C	268	CYS	2.0
1	D	303	ARG	2.0
1	D	438	VAL	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 [i](#)

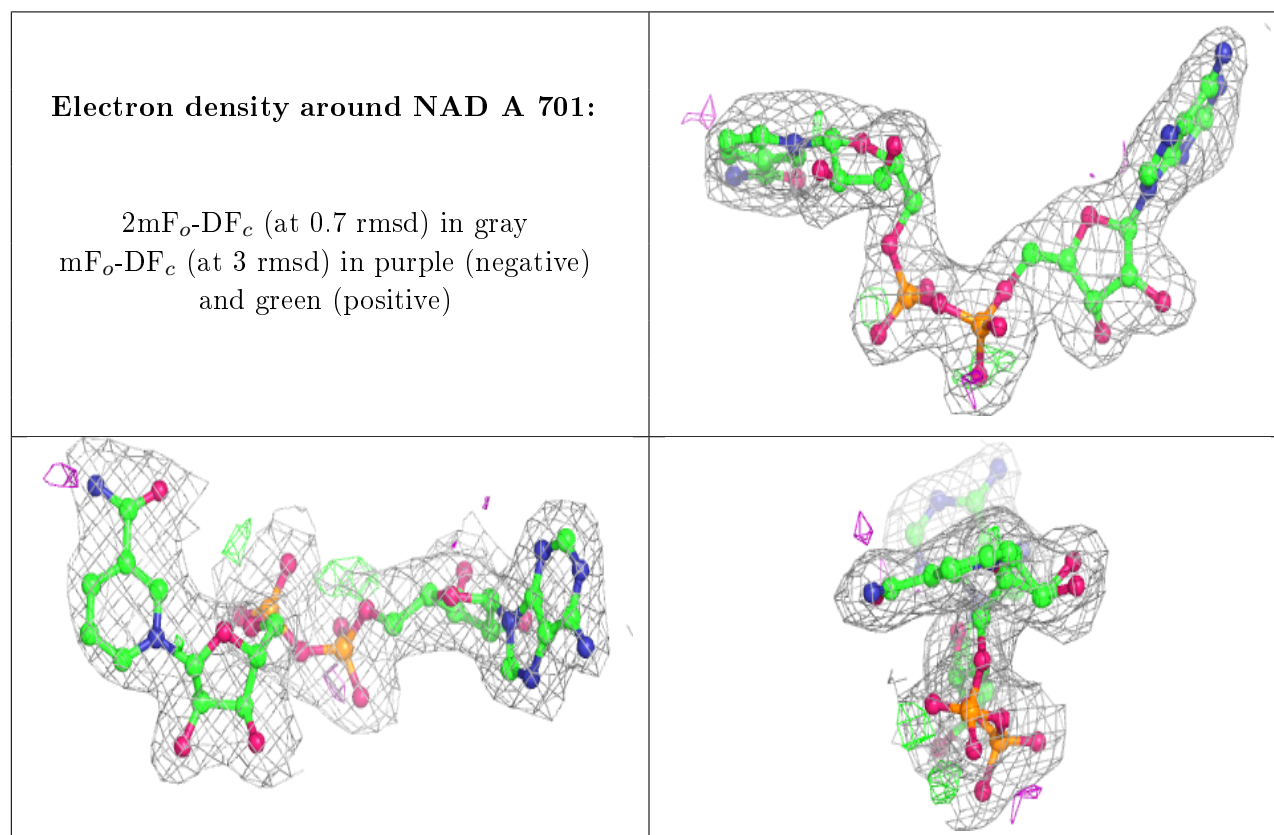
There are no carbohydrates in this entry.

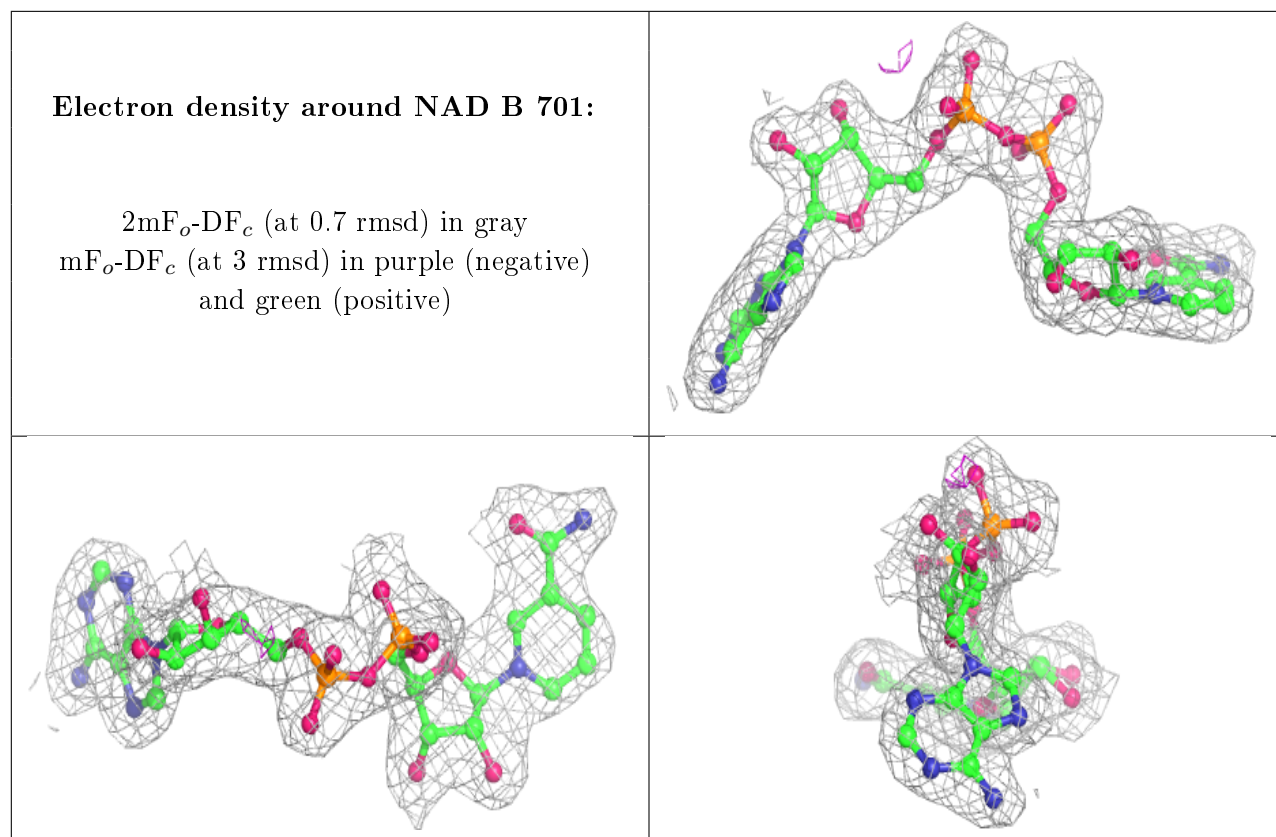
## 6.4 Ligands [i](#)

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
2	NAD	D	701[A]	44/44	0.92	0.16	57,74,80,179	9
2	NAD	C	701[A]	44/44	0.93	0.17	34,53,70,70	9
2	NAD	A	701	44/44	0.95	0.11	27,41,43,44	0
2	NAD	B	701	44/44	0.97	0.12	31,36,37,38	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.