



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 03:42 pm GMT

PDB ID : 4V37  
Title : Crystal structure of betaine aldehyde dehydrogenase from spinach showing a thiohemiacetal with 3-aminopropionaldehyde  
Authors : Zarate-Romero, A.; Munoz-Clares, R.A.  
Deposited on : 2014-10-16  
Resolution : 2.10 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

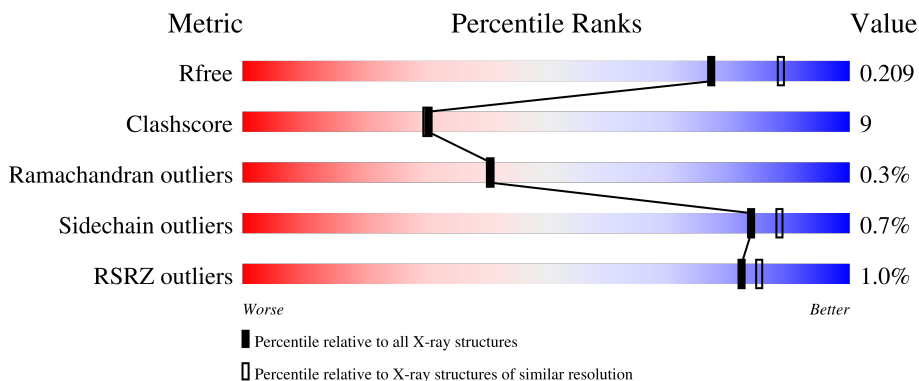
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



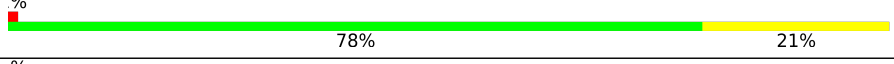

The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	497	
1	B	497	
1	C	497	
1	D	497	

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
5	PG4	A	1501	-	-	X	-
7	AE3	B	1501	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16821 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 BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	495	3852	2470	643	724	15	0	6	0
1	B	494	3846	2464	640	726	16	0	7	0
1	C	495	3856	2475	640	726	15	0	7	0
1	D	493	3838	2461	638	724	15	0	7	0

There are 4 discrepancies between the modelled and reference sequences:

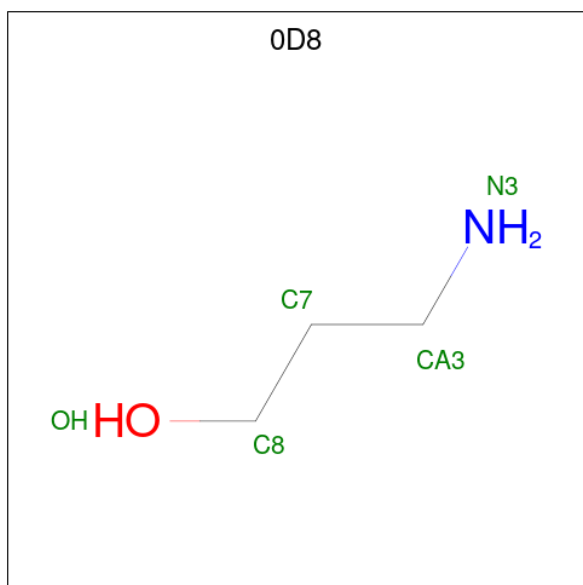
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	CYS	engineered mutation	UNP P17202
B	291	ALA	CYS	engineered mutation	UNP P17202
C	291	ALA	CYS	engineered mutation	UNP P17202
D	291	ALA	CYS	engineered mutation	UNP P17202

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



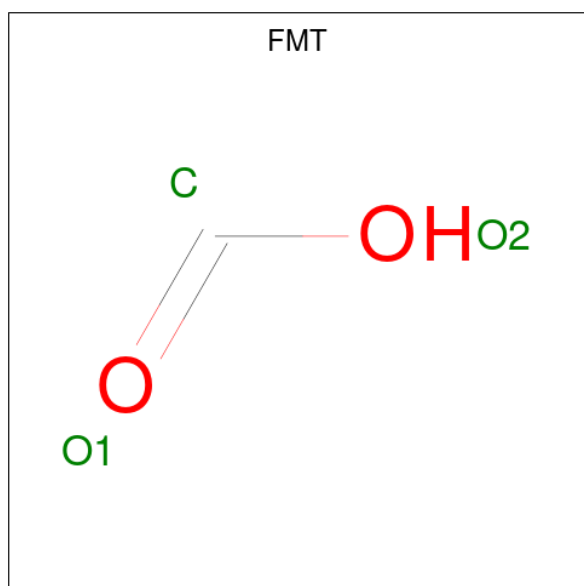
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	44	21	7	14	2	0	0
2	B	1	44	21	7	14	2	0	0
2	C	1	44	21	7	14	2	0	0
2	D	1	44	21	7	14	2	0	0

- Molecule 3 is 3-aminopropan-1-ol (three-letter code: OD8) (formula: C<sub>3</sub>H<sub>9</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).

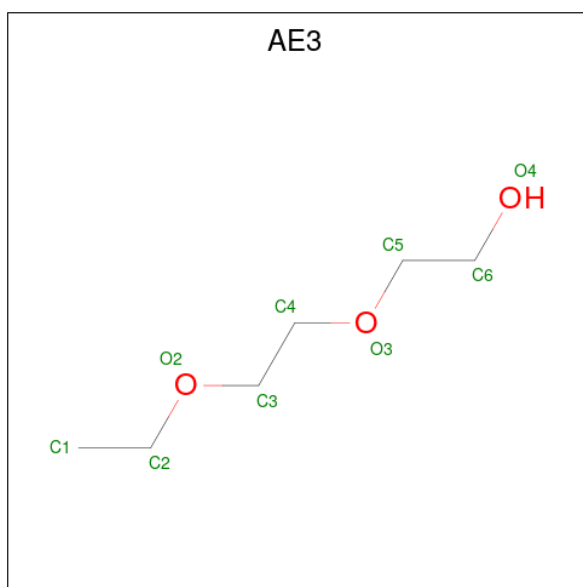


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 8 4	0	0
5	C	1	Total C O 12 8 4	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 7 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 8 is water.

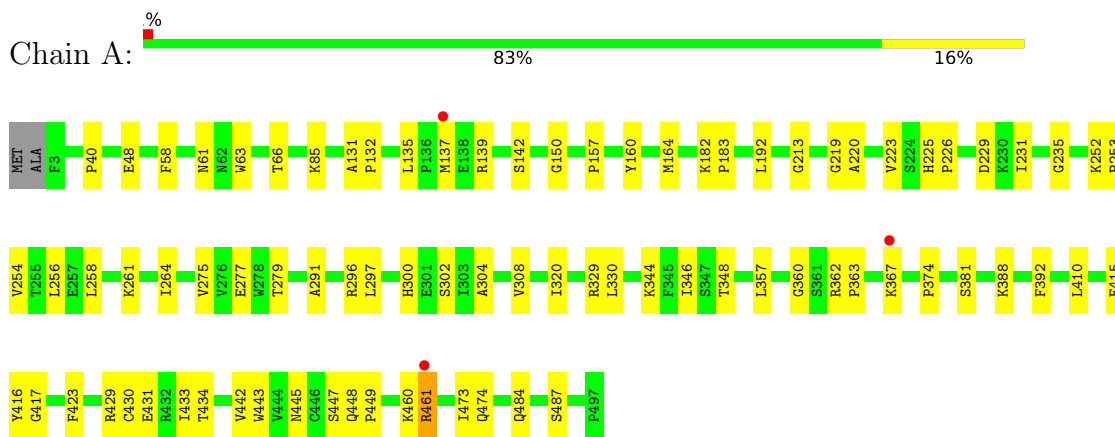
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	339	Total	O	0	0
			339	339		
8	B	278	Total	O	0	0
			278	278		
8	C	305	Total	O	0	0
			305	305		
8	D	257	Total	O	0	0
			257	257		



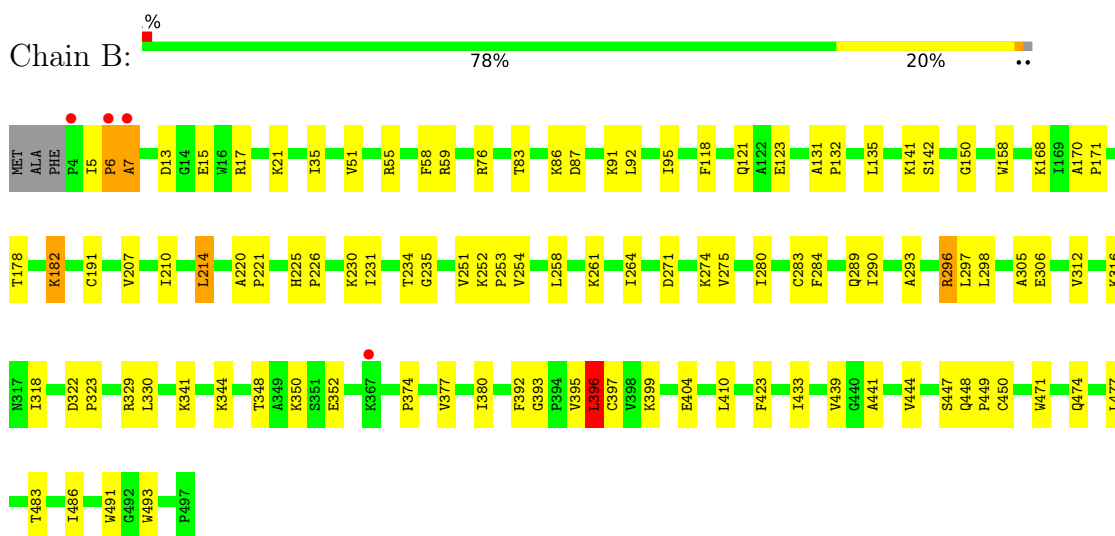
### 3 Residue-property plots [i](#)

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.

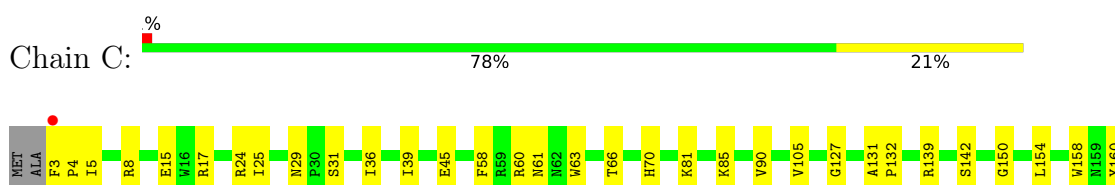
- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

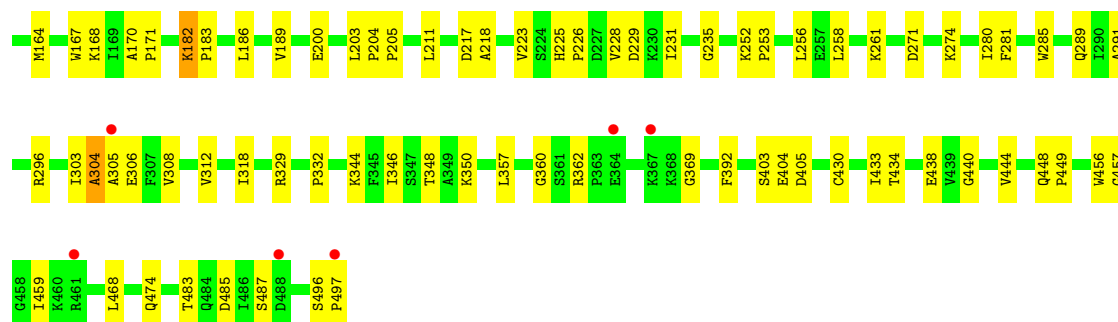


- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC

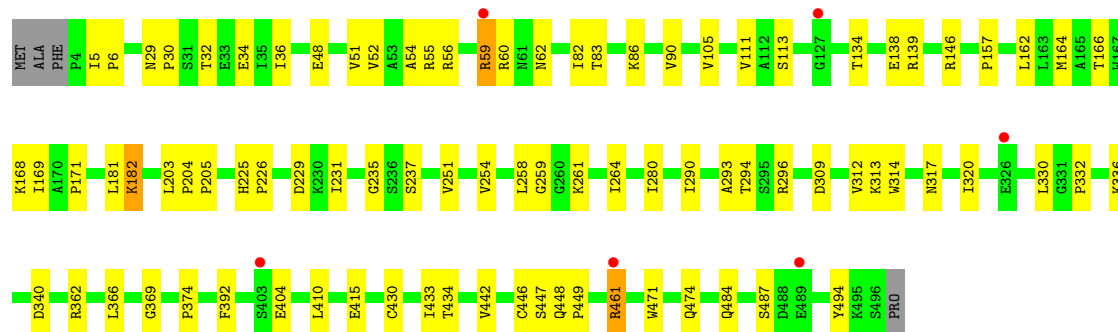
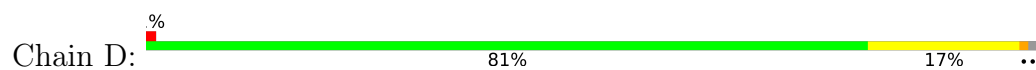


- Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC





● Molecule 1: BETAINE ALDEHYDE DEHYDROGENASE, CHLOROPLASTIC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.30Å 80.37Å 85.83Å 82.07° 86.40° 79.06°	Depositor
Resolution (Å)	24.48 – 2.10 24.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (24.48-2.10) 97.2 (24.48-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.167 , 0.209 0.169 , 0.209	Depositor DCC
$R_{free}$ test set	5048 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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, AE3, 0D8, PG4, FMT, K

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	0.54	1/3947 (0.0%)	0.61	0/5370
1	B	0.48	0/3940	0.62	6/5360 (0.1%)
1	C	0.46	0/3951	0.63	2/5379 (0.0%)
1	D	0.52	2/3931 (0.1%)	0.59	1/5349 (0.0%)
All	All	0.50	3/15769 (0.0%)	0.61	9/21458 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	6	PRO	N-CD	5.93	1.56	1.47
1	D	113	SER	CB-OG	-5.61	1.34	1.42
1	A	48	GLU	CD-OE2	-5.12	1.20	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	ALA	O-C-N	-13.54	101.04	122.70
1	B	7	ALA	N-CA-C	8.91	135.05	111.00
1	B	6	PRO	N-CA-C	8.42	133.99	112.10
1	B	6	PRO	CB-CA-C	-7.86	92.34	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	LEU	O-C-N	-6.91	111.64	122.70
1	C	304	ALA	CA-C-N	6.90	132.38	117.20
1	D	5	ILE	C-N-CD	5.20	139.31	128.40
1	B	296	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	214	LEU	CA-CB-CG	-5.18	103.38	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	396	LEU	Mainchain
1	B	7	ALA	Peptide
1	C	304	ALA	Peptide,Mainchain

## 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	3852	0	3849	66	0
1	B	3846	0	3838	91	0
1	C	3856	0	3856	78	0
1	D	3838	0	3838	68	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	25	2	0
2	D	44	0	26	1	0
3	A	5	0	8	0	0
3	B	5	0	8	1	0
3	C	10	0	17	2	0
3	D	5	0	8	0	0
4	A	3	0	1	0	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	3	0	1	0	0
5	A	12	0	15	7	0
5	C	12	0	15	2	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	9	0	14	8	0
8	A	339	0	0	11	0
8	B	278	0	0	13	0
8	C	305	0	0	6	0
8	D	257	0	0	2	0
All	All	16821	0	15573	288	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 9.

All (288) 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:B:121:GLN:NE2	8:B:2099:HOH:O	1.73	1.20
1:B:305[B]:ALA:O	8:B:2188:HOH:O	1.63	1.17
1:A:137:MET:HG2	8:A:2155:HOH:O	1.50	1.11
1:A:416:TYR:CE1	1:A:461:ARG:HD2	1.95	1.00
1:B:474[B]:GLN:NE2	8:B:2271:HOH:O	1.97	0.97
1:A:416:TYR:CD1	1:A:461:ARG:HD2	2.03	0.94
1:B:450:CYS:HB3	7:B:1501:AE3:H6C2	1.49	0.93
5:A:1501:PG4:H51	1:B:474[A]:GLN:HE22	1.36	0.89
1:C:430:CYS:O	1:C:434[A]:THR:HG23	1.72	0.87
1:C:403:SER:OG	1:C:405:ASP:OD1	1.94	0.86
7:B:1501:AE3:H1C3	8:B:2092:HOH:O	1.75	0.86
1:A:474:GLN:NE2	5:A:1501:PG4:H32	1.91	0.85
1:C:444:VAL:HB	1:D:484:GLN:HB3	1.59	0.84
1:A:223[A]:VAL:CG2	8:A:2194:HOH:O	2.27	0.81
1:B:17:ARG:NH1	8:B:2012:HOH:O	1.63	0.81
1:B:471:TRP:O	1:B:474[B]:GLN:HG3	1.80	0.81
1:B:449:PRO:HA	7:B:1501:AE3:H3C1	1.63	0.80
1:A:416:TYR:CE1	1:A:461:ARG:CD	2.67	0.77
7:B:1501:AE3:H5C1	8:B:2092:HOH:O	1.83	0.77
1:B:261:LYS:HG3	1:B:296:ARG:HD2	1.68	0.76
1:D:362:ARG:NH1	1:D:366:LEU:O	2.19	0.75
1:A:474:GLN:HE22	5:A:1501:PG4:H32	1.51	0.74
1:C:305[A]:ALA:HB3	8:C:2208:HOH:O	1.87	0.74
1:B:350:LYS:NZ	1:D:138:GLU:OE2	2.21	0.73
1:B:35:ILE:HD11	8:C:2023:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ALA:HB3	1:B:171:PRO:HD3	1.71	0.73
1:D:139:ARG:HG3	1:D:487:SER:HB3	1.71	0.73
5:A:1501:PG4:H51	1:B:474[A]:GLN:NE2	2.05	0.72
1:A:461:ARG:O	1:A:461:ARG:HG2	1.90	0.70
1:D:474:GLN:NE2	8:D:2113:HOH:O	2.25	0.70
1:A:223[A]:VAL:HG22	8:A:2194:HOH:O	1.92	0.69
1:D:56:ARG:HA	1:D:59:ARG:NH1	2.09	0.68
1:B:59:ARG:NH1	8:B:2043:HOH:O	2.27	0.68
1:A:415:GLU:HB2	1:A:461:ARG:HH21	1.59	0.68
1:A:304:ALA:O	1:A:308:VAL:HG12	1.95	0.67
1:B:251[A]:VAL:HG12	1:B:251[A]:VAL:O	1.95	0.67
1:B:5:ILE:HB	1:B:6:PRO:HD2	1.78	0.66
1:D:259:GLY:HA2	2:D:1497:NAD:O2D	1.95	0.66
1:C:256:LEU:HD12	1:D:251[B]:VAL:HG13	1.78	0.66
1:D:434[A]:THR:HG22	1:D:442:VAL:HG11	1.79	0.65
1:B:380:ILE:HG13	1:B:397[A]:CYS:HB2	1.79	0.65
1:B:289:GLN:HB3	1:B:392:PHE:CE2	2.32	0.65
1:C:449:PRO:HA	3:C:1500:OD8:HA21	1.80	0.64
1:D:32:THR:OG1	1:D:34:GLU:HG2	1.98	0.63
1:B:13:ASP:O	1:B:15:GLU:HG2	1.99	0.63
1:C:139:ARG:HG3	1:C:487:SER:HB3	1.79	0.63
1:C:256:LEU:CD1	1:D:251[B]:VAL:HG13	2.30	0.62
1:A:430:CYS:O	1:A:434[A]:THR:HG23	1.99	0.62
1:D:162:LEU:O	1:D:166[A]:THR:HG23	1.99	0.62
1:A:275:VAL:O	1:A:279:THR:HG23	1.99	0.61
1:D:251[B]:VAL:HG12	1:D:251[B]:VAL:O	2.00	0.61
1:D:55:ARG:O	1:D:59:ARG:HD3	2.00	0.61
1:D:261:LYS:HG3	1:D:296:ARG:HD2	1.82	0.61
1:C:8:ARG:O	1:C:24:ARG:NH2	2.23	0.61
1:C:303:ILE:O	1:C:305[A]:ALA:O	2.18	0.61
1:B:450:CYS:HB3	7:B:1501:AE3:C6	2.27	0.60
1:A:182:LYS:NZ	1:A:183:PRO:O	2.35	0.60
1:A:258:LEU:HD11	1:B:251[A]:VAL:HG11	1.84	0.60
1:B:450:CYS:H	7:B:1501:AE3:H3C1	1.65	0.60
1:A:434[A]:THR:HG21	8:A:2292:HOH:O	2.01	0.59
1:C:60:ARG:NH2	1:C:205:PRO:O	2.36	0.59
1:B:344:LYS:O	1:B:348:THR:HG23	2.02	0.59
1:D:362:ARG:NH2	1:D:369:GLY:O	2.36	0.59
1:A:258:LEU:CD1	1:B:251[A]:VAL:HG11	2.34	0.58
1:B:5:ILE:HB	1:B:6:PRO:CD	2.34	0.57
1:B:312:VAL:O	1:B:316:LYS:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:NH2	8:B:2008:HOH:O	2.02	0.57
1:C:362:ARG:NH2	1:C:369:GLY:O	2.38	0.57
1:C:85:LYS:NZ	1:C:200:GLU:OE1	2.38	0.57
1:D:415:GLU:HB3	1:D:461:ARG:HG3	1.87	0.57
1:B:377:VAL:HG12	1:B:380:ILE:HD11	1.86	0.56
1:B:21:LYS:HE2	1:C:61:ASN:HB3	1.86	0.56
1:D:237:SER:HA	1:D:258:LEU:HD13	1.87	0.56
1:C:127:GLY:HA3	8:C:2111:HOH:O	2.06	0.56
7:B:1501:AE3:H3C2	8:B:2092:HOH:O	2.05	0.56
1:B:491:TRP:O	8:B:2272:HOH:O	2.18	0.56
1:B:296:ARG:NH2	1:B:410:LEU:O	2.40	0.55
1:A:344:LYS:O	1:A:348:THR:HG23	2.06	0.55
1:D:146:ARG:NH1	1:D:474:GLN:HE22	2.03	0.55
1:C:142:SER:OG	1:C:483[A]:THR:HG22	2.06	0.55
1:A:300:HIS:ND1	1:A:302:SER:HB3	2.22	0.55
1:A:139:ARG:HG3	1:A:487:SER:HB3	1.88	0.55
1:C:29:ASN:HB2	1:C:36:ILE:HD13	1.89	0.55
1:B:214:LEU:HD13	1:C:70:HIS:HB2	1.89	0.55
1:B:312:VAL:HG12	1:B:316:LYS:HE2	1.89	0.55
1:C:258:LEU:CD1	1:D:251[B]:VAL:HG11	2.36	0.55
1:D:30:PRO:HB2	1:D:332:PRO:HG2	1.87	0.55
1:D:320:ILE:HG12	1:D:330:LEU:HD23	1.88	0.54
1:B:83:THR:O	1:B:86:LYS:HB2	2.07	0.54
1:B:450:CYS:CB	7:B:1501:AE3:H6C2	2.32	0.54
1:D:48:GLU:O	1:D:52:VAL:HG23	2.07	0.54
1:D:169:ILE:HD11	1:D:181:LEU:HD22	1.89	0.54
1:D:430:CYS:O	1:D:434[A]:THR:HG23	2.08	0.54
1:D:51[B]:VAL:O	1:D:52:VAL:C	2.43	0.54
1:D:474:GLN:HB2	8:D:2244:HOH:O	2.07	0.54
1:A:225:HIS:O	1:A:252:LYS:NZ	2.40	0.54
1:A:264:ILE:HG23	1:A:297:LEU:HA	1.90	0.54
1:C:154:LEU:HD22	1:C:168:LYS:HB3	1.90	0.53
1:D:261:LYS:HG3	1:D:296:ARG:CD	2.38	0.53
1:C:474:GLN:NE2	5:C:1502:PG4:H62	2.24	0.53
1:B:51:VAL:HG21	1:B:225:HIS:CE1	2.44	0.53
1:A:320:ILE:HG12	1:A:330:LEU:HD23	1.90	0.53
1:B:348:THR:HG22	1:D:134:THR:OG1	2.09	0.52
1:C:496:SER:HA	1:D:314:TRP:CH2	2.44	0.52
1:D:51[B]:VAL:O	1:D:54:ALA:N	2.42	0.52
1:D:264:ILE:HB	1:D:294:THR:HB	1.92	0.52
1:B:118:PHE:CZ	1:B:171:PRO:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:HG3	1:B:296:ARG:CD	2.39	0.52
1:B:142:SER:OG	1:B:483:THR:HG22	2.10	0.52
1:D:56:ARG:HA	1:D:59:ARG:HH11	1.75	0.51
1:A:434[A]:THR:HG22	1:A:442:VAL:HG11	1.93	0.51
1:B:404:GLU:HG3	1:B:433:ILE:HD11	1.92	0.51
1:D:330:LEU:HD22	1:D:374:PRO:HG3	1.93	0.51
1:A:296:ARG:NH2	1:A:410:LEU:O	2.43	0.51
1:A:362:ARG:HH21	1:A:367:LYS:C	2.14	0.51
1:B:230:LYS:HD3	1:B:253:PRO:HG2	1.93	0.51
1:C:182:LYS:HG2	1:C:211:LEU:O	2.11	0.51
1:C:308:VAL:O	1:C:312:VAL:HG13	2.10	0.51
1:A:61:ASN:OD1	1:A:61:ASN:N	2.41	0.51
1:D:231:ILE:HB	1:D:254:VAL:HG12	1.94	0.50
1:C:344:LYS:O	1:C:348:THR:HG23	2.12	0.50
1:D:60:ARG:C	1:D:62:ASN:H	2.14	0.50
5:A:1501:PG4:H52	8:A:2339:HOH:O	2.12	0.50
1:B:135:LEU:HD11	1:B:142:SER:HB2	1.92	0.50
1:B:158:TRP:CH2	1:B:392:PHE:HE2	2.30	0.50
1:C:182:LYS:HE2	1:C:182:LYS:C	2.32	0.50
1:C:63:TRP:O	1:C:66:THR:HG22	2.11	0.49
1:D:182:LYS:HD2	1:D:182:LYS:C	2.32	0.49
1:D:290:ILE:HB	1:D:293:ALA:HB2	1.93	0.49
1:C:329:ARG:NH2	8:C:2220:HOH:O	2.39	0.49
1:D:203:LEU:HD12	1:D:204:PRO:HD2	1.94	0.49
1:A:447:SER:C	1:A:449:PRO:HD3	2.33	0.49
1:C:228:VAL:O	1:C:252:LYS:HE2	2.12	0.49
1:B:76:ARG:NH1	1:B:123:GLU:OE2	2.31	0.49
5:C:1502:PG4:H21	1:D:471:TRP:CZ2	2.47	0.49
1:D:157:PRO:HG2	1:D:164:MET:HG3	1.94	0.49
1:A:431:GLU:HA	8:A:2292:HOH:O	2.12	0.49
1:D:296:ARG:NH2	1:D:410:LEU:O	2.46	0.49
1:B:182:LYS:HD2	1:B:182:LYS:C	2.33	0.48
1:A:235:GLY:O	1:A:258:LEU:HA	2.12	0.48
1:B:235:GLY:O	1:B:258:LEU:HA	2.13	0.48
1:C:182:LYS:HE2	1:C:183:PRO:O	2.13	0.48
1:B:298:LEU:HD23	1:B:399:LYS:HB3	1.95	0.48
1:D:51[A]:VAL:HG21	1:D:225:HIS:CE1	2.47	0.48
1:B:450:CYS:HB2	3:B:1499:OD8:H99	1.70	0.48
1:B:15:GLU:CD	1:B:17:ARG:HH21	2.17	0.48
1:C:280:ILE:HD13	1:C:318:ILE:HD11	1.95	0.48
1:A:484:GLN:CB	1:B:444:VAL:HB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ILE:HB	1:B:293:ALA:HB2	1.96	0.48
1:D:29:ASN:HB2	1:D:36:ILE:HD13	1.95	0.47
1:A:135:LEU:HD11	1:A:142:SER:HB2	1.94	0.47
1:B:474[B]:GLN:HA	1:B:477:LEU:HD12	1.95	0.47
1:A:357:LEU:HD13	8:A:2268:HOH:O	2.15	0.47
1:C:160:TYR:HB2	1:C:164:MET:HG2	1.95	0.47
1:A:443:TRP:CD1	1:A:449:PRO:HD2	2.50	0.47
1:C:3:PHE:HB2	1:C:4:PRO:HD3	1.96	0.47
1:B:178:THR:HG22	1:B:207:VAL:HA	1.97	0.47
1:C:305[A]:ALA:O	1:C:306[A]:GLU:CB	2.63	0.47
1:B:55:ARG:O	1:B:59:ARG:HG3	2.15	0.47
1:A:256:LEU:CD1	1:B:251[A]:VAL:HG13	2.46	0.46
1:C:182:LYS:CE	1:C:183:PRO:O	2.63	0.46
1:A:330:LEU:HD22	1:A:374:PRO:HG3	1.97	0.46
1:A:346:ILE:HD13	1:A:360:GLY:HA2	1.98	0.46
1:C:167:TRP:CG	1:C:468:LEU:HD21	2.50	0.46
1:C:305[A]:ALA:O	1:C:306[A]:GLU:HB3	2.15	0.46
1:A:85:LYS:NZ	8:A:2106:HOH:O	2.48	0.46
1:B:280:ILE:HG21	1:B:318:ILE:HD11	1.98	0.46
1:C:312:VAL:CG1	1:C:357:LEU:HD21	2.45	0.46
1:C:350:LYS:HA	1:C:350:LYS:HD3	1.65	0.46
1:A:220:ALA:O	1:A:223[A]:VAL:HG22	2.15	0.46
1:C:261:LYS:HG3	1:C:296:ARG:CD	2.46	0.46
1:C:235:GLY:O	1:C:258:LEU:HA	2.16	0.46
1:C:252:LYS:HB2	1:C:252:LYS:HE3	1.59	0.45
1:B:393:GLY:O	1:B:395:VAL:N	2.48	0.45
1:B:439:VAL:HG13	1:B:441:ALA:H	1.81	0.45
1:C:158:TRP:CD1	1:C:186:LEU:HD12	2.51	0.45
1:A:261:LYS:HG3	1:A:296:ARG:CD	2.47	0.45
1:B:141:LYS:HD3	1:B:486:ILE:HD13	1.98	0.45
1:B:330:LEU:HD22	1:B:374:PRO:HG3	1.98	0.45
1:C:456:TRP:CZ3	3:C:1499:OD8:H89	2.51	0.45
1:D:225:HIS:HA	1:D:226:PRO:HD3	1.85	0.45
1:B:131:ALA:HA	1:B:132:PRO:HD3	1.84	0.45
1:B:275:VAL:HG22	1:B:423:PHE:CD2	2.52	0.45
1:B:474[A]:GLN:HA	1:B:477:LEU:HD12	1.98	0.44
1:D:83:THR:O	1:D:86:LYS:HB2	2.17	0.44
1:A:429:ARG:O	1:A:433:ILE:HG12	2.17	0.44
1:C:258:LEU:HD11	1:D:251[B]:VAL:HG11	1.98	0.44
1:D:404:GLU:HG3	1:D:433:ILE:HD11	2.00	0.44
1:D:82:ILE:HG21	1:D:111:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:GLU:O	1:D:461:ARG:HB2	2.18	0.44
1:B:447:SER:C	1:B:449:PRO:HD3	2.38	0.44
1:C:45:GLU:HG2	8:C:2040:HOH:O	2.17	0.44
1:A:229:ASP:O	1:A:253:PRO:HD2	2.18	0.44
1:A:434[A]:THR:CG2	8:A:2292:HOH:O	2.62	0.44
1:C:261:LYS:HG3	1:C:296:ARG:HD2	1.99	0.44
1:C:31:SER:HA	1:C:332:PRO:HG3	1.99	0.44
1:C:312:VAL:HG11	1:C:357:LEU:HD21	1.98	0.44
1:B:283:CYS:SG	1:B:396:LEU:HB2	2.58	0.43
1:A:182:LYS:HD2	1:A:219:GLY:N	2.33	0.43
1:A:388:LYS:NZ	8:A:2270:HOH:O	2.33	0.43
1:B:87:ASP:HB2	8:B:2074:HOH:O	2.18	0.43
1:A:329:ARG:HD3	1:A:329:ARG:HA	1.70	0.43
1:A:277:GLU:OE2	1:B:493:TRP:N	2.49	0.43
1:A:362:ARG:HA	1:A:363:PRO:HD3	1.91	0.43
1:C:170:ALA:HB3	1:C:171:PRO:HD3	1.99	0.43
1:D:309:ASP:O	1:D:312:VAL:HG22	2.18	0.43
1:D:447:SER:O	1:D:449:PRO:HD3	2.18	0.43
1:A:231:ILE:HB	1:A:254:VAL:HG12	2.00	0.43
1:C:392:PHE:CE1	2:C:1498:NAD:H2D	2.54	0.43
1:D:90[B]:VAL:HG11	1:D:105:VAL:HG12	2.00	0.43
1:B:91:LYS:HB2	1:B:91:LYS:HE3	1.60	0.43
1:A:58:PHE:CE1	1:A:150:GLY:HA2	2.54	0.43
5:A:1501:PG4:H31	8:A:2339:HOH:O	2.18	0.43
1:C:25[A]:ILE:HG13	1:C:39:ILE:HG13	1.99	0.43
1:A:460:LYS:HB3	1:A:461:ARG:H	1.51	0.43
1:B:261:LYS:CG	1:B:296:ARG:HD2	2.43	0.43
1:B:264:ILE:HG23	1:B:297:LEU:HA	2.01	0.43
1:D:280:ILE:CD1	1:D:314:TRP:HB3	2.49	0.43
1:A:58:PHE:CZ	1:A:150:GLY:HA2	2.54	0.42
1:A:423:PHE:CD2	1:A:445:ASN:HA	2.54	0.42
1:B:341:LYS:HD2	8:B:2202:HOH:O	2.18	0.42
1:C:223:VAL:HB	1:C:231:ILE:HG13	2.00	0.42
1:C:485:ASP:HB2	1:D:446:CYS:HB3	2.01	0.42
1:A:225:HIS:HA	1:A:226:PRO:HD3	1.87	0.42
1:C:438:GLU:C	1:C:459:ILE:HD11	2.40	0.42
1:B:225:HIS:O	1:B:252:LYS:NZ	2.52	0.42
1:C:496:SER:HA	1:D:314:TRP:CZ3	2.55	0.42
1:D:51[A]:VAL:HG21	1:D:225:HIS:NE2	2.35	0.42
1:C:404:GLU:HG3	1:C:433:ILE:HD11	2.01	0.42
5:A:1501:PG4:H52	5:A:1501:PG4:H31	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ILE:HD13	1:C:360:GLY:HA2	2.01	0.42
1:A:291:ALA:HB2	2:A:1498:NAD:C2N	2.50	0.42
1:C:5:ILE:HD13	1:C:189:VAL:HG21	2.01	0.42
1:C:229:ASP:O	1:C:253:PRO:HD2	2.19	0.42
1:A:131:ALA:HA	1:A:132:PRO:HD3	1.94	0.42
1:B:231:ILE:HB	1:B:254:VAL:HG12	2.01	0.42
1:C:182:LYS:HE2	1:C:182:LYS:O	2.19	0.42
1:C:203[B]:LEU:HD12	1:C:204:PRO:HD2	2.01	0.42
1:C:497:PRO:HD2	1:D:317:ASN:ND2	2.35	0.42
1:B:271:ASP:OD2	1:B:274:LYS:HE2	2.19	0.41
1:B:280:ILE:HG23	1:B:284:PHE:HD2	1.85	0.41
1:C:289:GLN:HB3	1:C:392:PHE:CE2	2.55	0.41
1:B:15:GLU:OE2	1:B:17:ARG:NH2	2.53	0.41
1:B:86:LYS:HB3	1:B:86:LYS:HE2	1.80	0.41
1:C:280:ILE:HG22	1:D:494:TYR:CE2	2.54	0.41
1:D:280:ILE:HD11	1:D:314:TRP:HB3	2.02	0.41
1:A:63:TRP:O	1:A:66:THR:HG22	2.19	0.41
1:B:348:THR:O	1:B:352:GLU:HG3	2.19	0.41
1:C:90:VAL:HG11	1:C:105:VAL:HG12	2.01	0.41
1:C:131:ALA:HA	1:C:132:PRO:HD3	1.87	0.41
1:D:55:ARG:NH2	1:D:229:ASP:OD2	2.51	0.41
1:D:60:ARG:HB3	1:D:62:ASN:HB2	2.01	0.41
1:D:168:LYS:O	1:D:171:PRO:HD2	2.20	0.41
1:D:235:GLY:O	1:D:258:LEU:HA	2.20	0.41
1:B:329:ARG:HD3	1:B:329:ARG:HA	1.83	0.41
1:D:309:ASP:OD1	1:D:313:LYS:NZ	2.36	0.41
1:A:157:PRO:HG2	1:A:164:MET:HG3	2.01	0.41
1:A:415:GLU:O	1:A:460:LYS:HB3	2.21	0.41
1:B:225:HIS:HA	1:B:226:PRO:HD3	1.93	0.41
1:C:271:ASP:OD2	1:C:274:LYS:HE2	2.20	0.41
1:A:474:GLN:H	1:A:474:GLN:HG2	1.65	0.41
1:C:291:ALA:HB2	2:C:1498:NAD:C2N	2.51	0.41
1:C:225:HIS:HA	1:C:226:PRO:HD3	1.98	0.41
1:A:40:PRO:HD2	1:A:192:LEU:HD11	2.03	0.41
1:A:182:LYS:HE2	1:A:213:GLY:O	2.21	0.41
1:B:191:CYS:O	1:B:210:ILE:HD13	2.21	0.41
1:B:322:ASP:HA	1:B:323:PRO:HD3	1.93	0.41
1:C:15:GLU:HG3	1:C:17:ARG:HD3	2.03	0.41
1:C:182:LYS:HD2	1:C:218:ALA:HB3	2.01	0.41
1:C:440:GLY:HA3	1:C:457:GLY:O	2.20	0.41
1:D:204:PRO:HA	1:D:205:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:LYS:HE2	1:D:340:ASP:OD1	2.21	0.41
1:A:484:GLN:HB3	1:B:444:VAL:HB	2.03	0.41
1:B:168:LYS:NZ	1:B:234:THR:OG1	2.43	0.41
1:B:17:ARG:NH1	8:B:2008:HOH:O	2.54	0.40
1:C:204:PRO:HA	1:C:205:PRO:HD3	1.92	0.40
1:C:281:PHE:O	1:C:285:TRP:HB3	2.21	0.40
1:B:92:LEU:O	1:B:95:ILE:HG22	2.21	0.40
1:C:60:ARG:NH2	8:C:2057:HOH:O	2.29	0.40
1:A:160:TYR:HB2	1:A:164:MET:HG2	2.03	0.40
1:B:220:ALA:HB3	1:B:221:PRO:HD3	2.04	0.40
1:C:81:LYS:HD2	1:C:81:LYS:HA	1.93	0.40
1:D:90[B]:VAL:HG22	1:D:105:VAL:HA	2.02	0.40
1:A:416:TYR:O	1:A:460:LYS:HD3	2.21	0.40
1:B:251[A]:VAL:O	1:B:251[A]:VAL:CG1	2.67	0.40
1:C:58:PHE:CE1	1:C:150:GLY:HA2	2.56	0.40
1:A:256:LEU:HD12	1:B:251[A]:VAL:HG13	2.04	0.40
1:B:58:PHE:CE1	1:B:150:GLY:HA2	2.57	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	499/497 (100%)	482 (97%)	15 (3%)	2 (0%)	34 32
1	B	499/497 (100%)	479 (96%)	17 (3%)	3 (1%)	25 21
1	C	500/497 (101%)	479 (96%)	20 (4%)	1 (0%)	47 49
1	D	498/497 (100%)	474 (95%)	23 (5%)	1 (0%)	47 49
All	All	1996/1988 (100%)	1914 (96%)	75 (4%)	7 (0%)	41 32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	GLN
1	B	306[A]	GLU
1	B	306[B]	GLU
1	B	448	GLN
1	C	448	GLN
1	D	448	GLN
1	A	417	GLY

### 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	414/409 (101%)	410 (99%)	4 (1%)	76 82
1	B	413/409 (101%)	412 (100%)	1 (0%)	93 96
1	C	414/409 (101%)	412 (100%)	2 (0%)	88 92
1	D	413/409 (101%)	409 (99%)	4 (1%)	76 82
All	All	1654/1636 (101%)	1643 (99%)	11 (1%)	84 88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	SER
1	A	392	PHE
1	A	461	ARG
1	A	473	ILE
1	B	182	LYS
1	C	182	LYS
1	C	217	ASP
1	D	59	ARG
1	D	182	LYS
1	D	392	PHE
1	D	461	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	474	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](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

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	OD8	D	1498	1	4,4,4	0.21	0	3,3,3	0.65	0
2	NAD	B	1498	-	42,48,48	2.00	16 (38%)	50,73,73	1.56	11 (22%)
5	PG4	A	1501	-	11,11,12	0.69	0	10,10,11	0.85	0
3	OD8	C	1500	-	4,4,4	0.67	0	3,3,3	1.70	1 (33%)
2	NAD	A	1498	-	42,48,48	1.82	15 (35%)	50,73,73	1.75	10 (20%)
2	NAD	D	1497	-	42,48,48	1.81	12 (28%)	50,73,73	1.31	6 (12%)
2	NAD	C	1498	-	42,48,48	1.91	15 (35%)	50,73,73	1.77	11 (22%)
4	FMT	B	1500	-	2,2,2	0.69	0	1,1,1	0.62	0
7	AE3	B	1501	-	8,8,8	0.29	0	7,7,7	0.97	1 (14%)
5	PG4	C	1502	-	11,11,12	0.50	0	10,10,11	0.99	0
4	FMT	C	1501	-	2,2,2	0.69	0	1,1,1	0.62	0
3	OD8	C	1499	1	4,4,4	0.21	0	3,3,3	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	0D8	B	1499	1	4,4,4	0.19	0	3,3,3	0.69	0
3	0D8	A	1499	1	4,4,4	0.23	0	3,3,3	1.06	0
4	FMT	A	1500	-	2,2,2	0.68	0	1,1,1	0.62	0
4	FMT	D	1499	-	2,2,2	0.68	0	1,1,1	0.61	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	0D8	D	1498	1	-	1/2/2/2	-
2	NAD	B	1498	-	-	1/26/62/62	0/5/5/5
5	PG4	A	1501	-	-	4/9/9/10	-
3	0D8	C	1500	-	-	1/2/2/2	-
2	NAD	A	1498	-	-	1/26/62/62	0/5/5/5
2	NAD	D	1497	-	-	1/26/62/62	0/5/5/5
2	NAD	C	1498	-	-	1/26/62/62	0/5/5/5
7	AE3	B	1501	-	-	3/6/6/6	-
5	PG4	C	1502	-	-	5/9/9/10	-
3	0D8	C	1499	1	-	0/2/2/2	-
3	0D8	B	1499	1	-	1/2/2/2	-
3	0D8	A	1499	1	-	0/2/2/2	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1497	NAD	PA-O2A	-4.08	1.36	1.55
2	B	1498	NAD	PN-O2N	-3.97	1.36	1.55
2	A	1498	NAD	PN-O2N	-3.83	1.37	1.55
2	C	1498	NAD	O4D-C4D	-3.71	1.36	1.45
2	D	1497	NAD	PN-O2N	-3.70	1.38	1.55
2	C	1498	NAD	PN-O2N	-3.68	1.38	1.55
2	B	1498	NAD	PA-O1A	-3.66	1.37	1.50
2	C	1498	NAD	O7N-C7N	-3.47	1.17	1.24
2	B	1498	NAD	O4B-C4B	-3.46	1.37	1.45
2	D	1497	NAD	O7N-C7N	-3.44	1.17	1.24
2	A	1498	NAD	PA-O2A	-3.42	1.39	1.55
2	A	1498	NAD	PA-O1A	-3.39	1.38	1.50
2	B	1498	NAD	PA-O2A	-3.30	1.39	1.55
2	D	1497	NAD	PA-O1A	-3.19	1.39	1.50
2	B	1498	NAD	C5A-N7A	-3.18	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1498	NAD	C4A-N3A	-3.12	1.31	1.35
2	D	1497	NAD	C2N-N1N	-3.12	1.31	1.35
2	C	1498	NAD	PA-O1A	-3.12	1.39	1.50
2	B	1498	NAD	O7N-C7N	-3.07	1.18	1.24
2	B	1498	NAD	PN-O1N	-2.97	1.40	1.50
2	A	1498	NAD	O4B-C1B	-2.97	1.36	1.41
2	C	1498	NAD	O4B-C4B	-2.96	1.38	1.45
2	B	1498	NAD	C2N-N1N	-2.96	1.31	1.35
2	A	1498	NAD	O4B-C4B	-2.92	1.38	1.45
2	C	1498	NAD	O3D-C3D	-2.84	1.36	1.43
2	A	1498	NAD	PN-O1N	-2.82	1.40	1.50
2	C	1498	NAD	PN-O1N	-2.81	1.41	1.50
2	D	1497	NAD	C5A-N7A	-2.80	1.29	1.39
2	C	1498	NAD	C4A-N3A	-2.79	1.31	1.35
2	D	1497	NAD	O4D-C4D	-2.78	1.38	1.45
2	C	1498	NAD	PA-O2A	-2.73	1.42	1.55
2	D	1497	NAD	PN-O1N	-2.68	1.41	1.50
2	B	1498	NAD	O4D-C1D	-2.64	1.37	1.41
2	A	1498	NAD	C2N-N1N	-2.61	1.31	1.35
2	A	1498	NAD	O3D-C3D	-2.59	1.36	1.43
2	D	1497	NAD	O4B-C4B	-2.59	1.39	1.45
2	C	1498	NAD	C2B-C1B	-2.56	1.49	1.53
2	B	1498	NAD	O2D-C2D	-2.56	1.37	1.43
2	A	1498	NAD	C5A-N7A	-2.54	1.30	1.39
2	C	1498	NAD	C5A-N7A	-2.51	1.30	1.39
2	A	1498	NAD	O7N-C7N	-2.51	1.19	1.24
2	C	1498	NAD	O2B-C2B	-2.49	1.37	1.43
2	B	1498	NAD	O4D-C4D	-2.37	1.39	1.45
2	B	1498	NAD	O3D-C3D	-2.31	1.37	1.43
2	A	1498	NAD	O4D-C1D	-2.30	1.37	1.41
2	A	1498	NAD	O4D-C4D	-2.30	1.39	1.45
2	C	1498	NAD	C7N-N7N	-2.26	1.28	1.33
2	B	1498	NAD	C2B-C1B	-2.22	1.50	1.53
2	A	1498	NAD	O3B-C3B	-2.21	1.37	1.43
2	B	1498	NAD	O2B-C2B	-2.15	1.37	1.43
2	D	1497	NAD	C4A-N3A	-2.14	1.32	1.35
2	C	1498	NAD	O3B-C3B	-2.13	1.38	1.43
2	A	1498	NAD	O2B-C2B	-2.12	1.38	1.43
2	A	1498	NAD	C7N-N7N	-2.09	1.29	1.33
2	B	1498	NAD	C6N-N1N	-2.09	1.30	1.35
2	C	1498	NAD	O2D-C2D	-2.07	1.38	1.43
2	D	1497	NAD	O2B-C2B	-2.03	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1497	NAD	O4B-C1B	-2.02	1.38	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1498	NAD	N3A-C2A-N1A	-4.73	121.28	128.68
2	C	1498	NAD	O7N-C7N-C3N	4.44	124.94	119.63
2	A	1498	NAD	C3N-C2N-N1N	4.20	124.53	120.43
2	C	1498	NAD	O7N-C7N-N7N	-3.97	116.94	122.58
2	C	1498	NAD	N3A-C2A-N1A	-3.94	122.53	128.68
2	A	1498	NAD	O7N-C7N-N7N	-3.76	117.23	122.58
2	C	1498	NAD	C4A-C5A-N7A	-3.66	105.58	109.40
2	D	1497	NAD	N3A-C2A-N1A	-3.55	123.13	128.68
2	B	1498	NAD	C4A-C5A-N7A	-3.44	105.81	109.40
2	B	1498	NAD	C2A-N1A-C6A	3.41	124.59	118.75
2	D	1497	NAD	C4A-C5A-N7A	-3.40	105.86	109.40
2	A	1498	NAD	C6N-N1N-C2N	-3.32	118.95	121.97
2	C	1498	NAD	C3N-C2N-N1N	3.13	123.49	120.43
2	C	1498	NAD	C1B-N9A-C4A	-3.10	121.19	126.64
2	A	1498	NAD	C2A-N1A-C6A	3.09	124.04	118.75
2	B	1498	NAD	N3A-C2A-N1A	-2.93	124.10	128.68
2	A	1498	NAD	C4A-C5A-N7A	-2.90	106.38	109.40
2	C	1498	NAD	C5D-C4D-C3D	-2.88	104.39	115.18
2	C	1498	NAD	C2A-N1A-C6A	2.87	123.67	118.75
2	A	1498	NAD	O4B-C4B-C3B	2.80	110.66	105.11
2	B	1498	NAD	C3N-C2N-N1N	2.68	123.04	120.43
2	D	1497	NAD	C2A-N1A-C6A	2.62	123.24	118.75
2	B	1498	NAD	C5D-C4D-C3D	-2.59	105.47	115.18
3	C	1500	0D8	CA3-C7-C8	-2.51	108.97	112.89
2	B	1498	NAD	O2N-PN-O5D	-2.47	96.25	107.75
2	C	1498	NAD	C5A-C6A-N6A	2.44	124.06	120.35
2	A	1498	NAD	C5N-C4N-C3N	-2.44	117.46	120.34
2	A	1498	NAD	O7N-C7N-C3N	2.40	122.51	119.63
2	D	1497	NAD	C5N-C4N-C3N	-2.35	117.56	120.34
2	B	1498	NAD	O4B-C4B-C3B	2.33	109.72	105.11
2	B	1498	NAD	C5A-C6A-N1A	-2.28	115.19	120.35
2	D	1497	NAD	C1B-N9A-C4A	-2.24	122.70	126.64
2	B	1498	NAD	O2N-PN-O1N	2.24	123.30	112.24
2	B	1498	NAD	C1B-N9A-C4A	-2.18	122.82	126.64
2	B	1498	NAD	O7N-C7N-C3N	2.18	122.24	119.63
2	D	1497	NAD	C5A-C6A-N6A	2.14	123.61	120.35
2	C	1498	NAD	O4B-C4B-C3B	2.06	109.19	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1501	AE3	O3-C4-C3	-2.04	101.22	110.39
2	A	1498	NAD	C3N-C7N-N7N	2.02	120.18	117.75
2	C	1498	NAD	C3B-C2B-C1B	2.00	103.99	100.98

There are no chirality outliers.

All (19) torsion outliers are listed below:

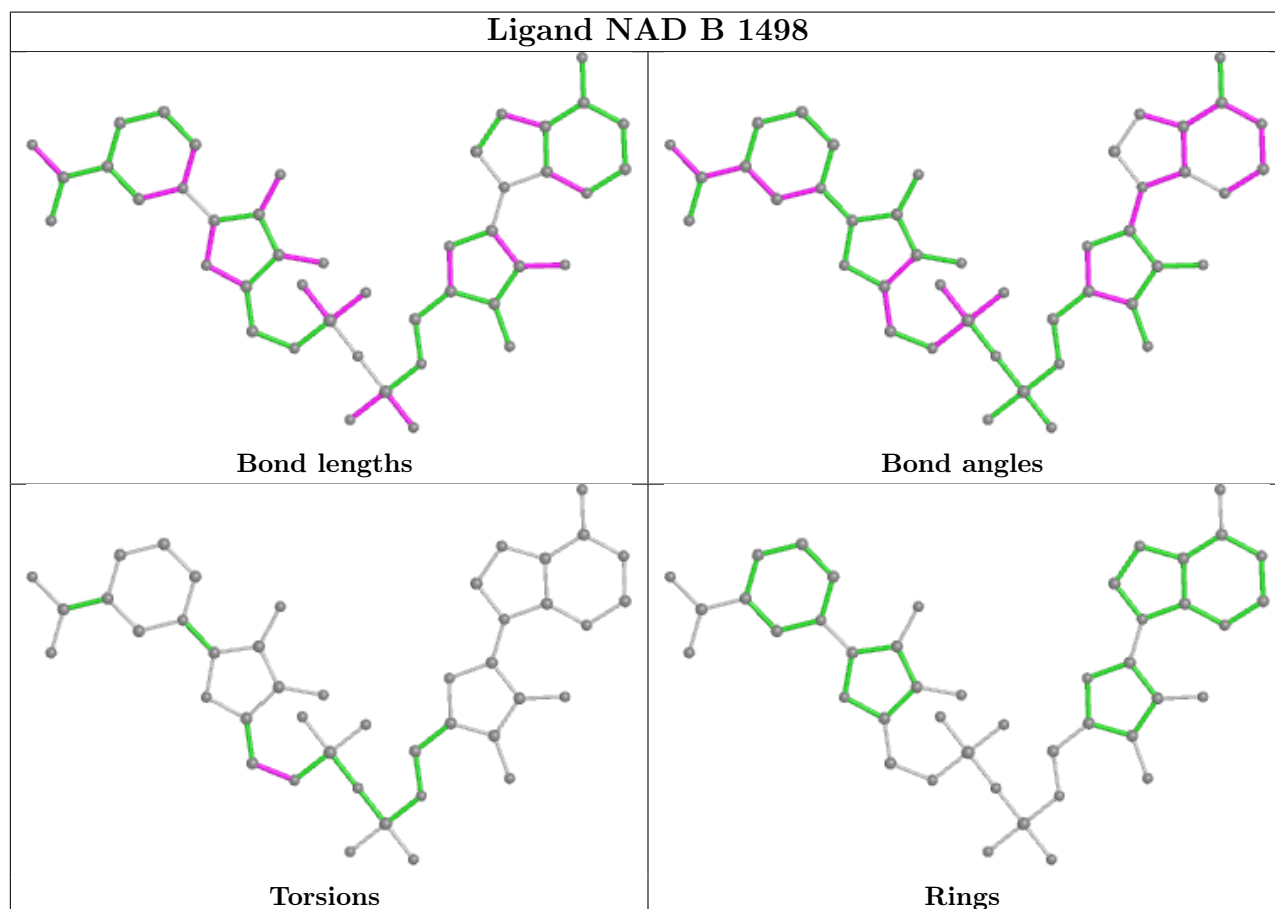
Mol	Chain	Res	Type	Atoms
5	A	1501	PG4	C3-C4-O3-C5
5	C	1502	PG4	O2-C3-C4-O3
3	D	1498	0D8	CA3-C7-C8-OH
5	C	1502	PG4	O3-C5-C6-O4
5	A	1501	PG4	O1-C1-C2-O2
5	C	1502	PG4	O1-C1-C2-O2
7	B	1501	AE3	O3-C5-C6-O4
3	B	1499	0D8	CA3-C7-C8-OH
2	A	1498	NAD	C4D-C5D-O5D-PN
2	C	1498	NAD	C4D-C5D-O5D-PN
2	D	1497	NAD	C4D-C5D-O5D-PN
5	C	1502	PG4	C5-C6-O4-C7
2	B	1498	NAD	C4D-C5D-O5D-PN
5	C	1502	PG4	C3-C4-O3-C5
7	B	1501	AE3	C1-C2-O2-C3
3	C	1500	0D8	C8-C7-CA3-N3
5	A	1501	PG4	O3-C5-C6-O4
7	B	1501	AE3	O2-C3-C4-O3
5	A	1501	PG4	O2-C3-C4-O3

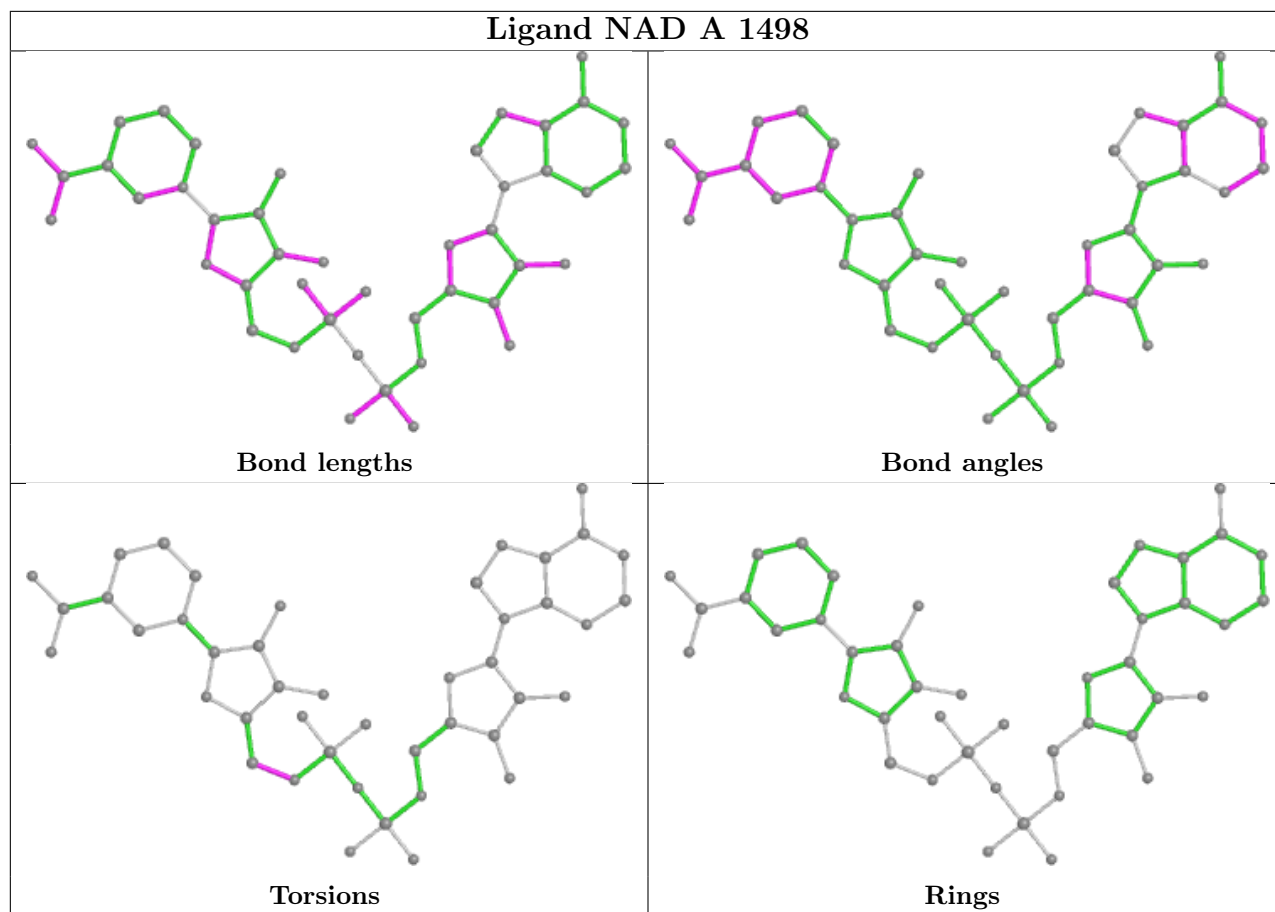
There are no ring outliers.

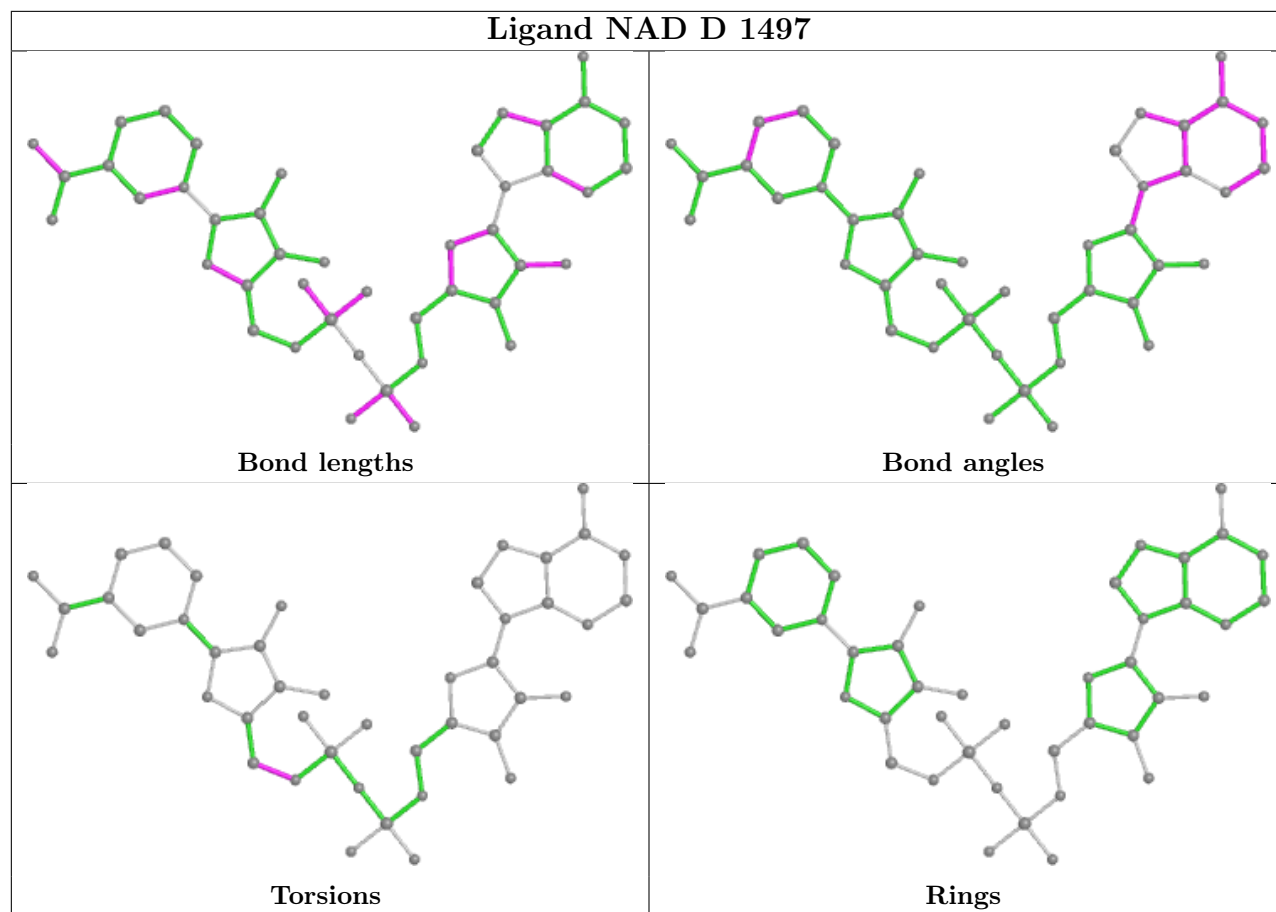
9 monomers are involved in 24 short contacts:

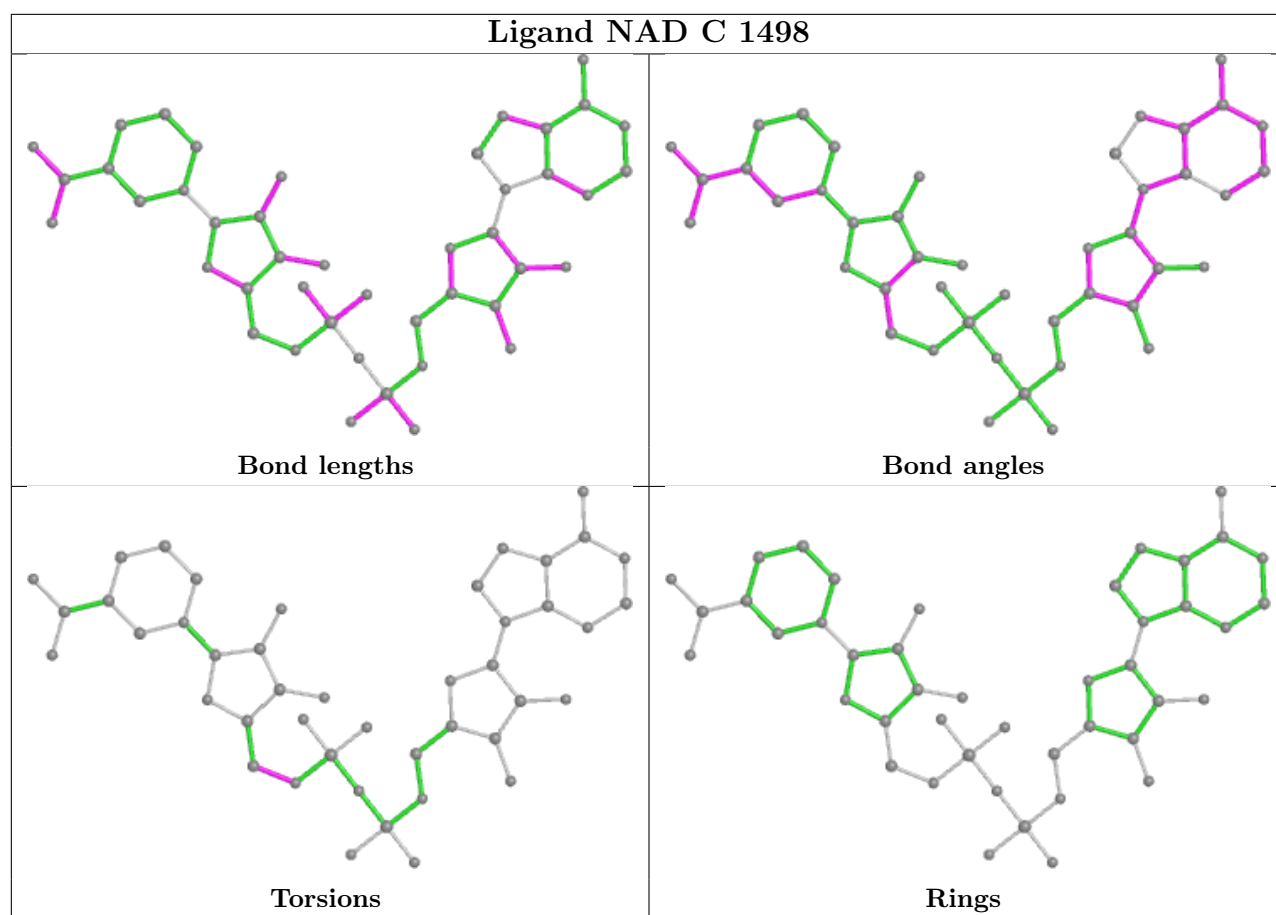
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1501	PG4	7	0
3	C	1500	0D8	1	0
2	A	1498	NAD	1	0
2	D	1497	NAD	1	0
2	C	1498	NAD	2	0
7	B	1501	AE3	8	0
5	C	1502	PG4	2	0
3	C	1499	0D8	1	0
3	B	1499	0D8	1	0

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 [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	495/497 (99%)	-0.21	3 (0%) 89 91	9, 19, 36, 60	0
1	B	494/497 (99%)	-0.16	4 (0%) 86 88	11, 20, 36, 79	0
1	C	495/497 (99%)	-0.10	7 (1%) 75 78	11, 23, 45, 68	0
1	D	493/497 (99%)	-0.09	6 (1%) 79 82	11, 23, 41, 55	0
All	All	1977/1988 (99%)	-0.14	20 (1%) 82 85	9, 21, 40, 79	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	PRO	6.7
1	C	497	PRO	3.9
1	C	3	PHE	3.4
1	B	367	LYS	3.3
1	D	127	GLY	3.2
1	D	326	GLU	3.1
1	C	305[A]	ALA	2.8
1	C	367	LYS	2.7
1	D	403	SER	2.6
1	C	364	GLU	2.6
1	B	7	ALA	2.6
1	A	461	ARG	2.5
1	A	137	MET	2.3
1	D	489	GLU	2.3
1	D	59	ARG	2.3
1	D	461	ARG	2.2
1	B	6	PRO	2.1
1	C	461	ARG	2.1
1	C	488	ASP	2.1
1	A	367	LYS	2.0



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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

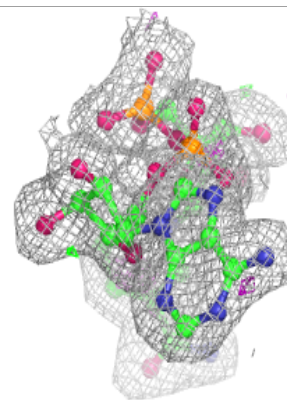
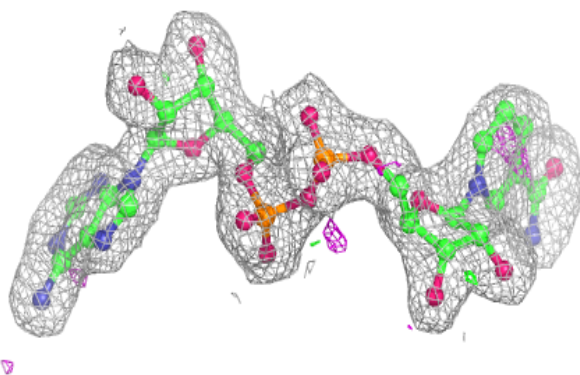
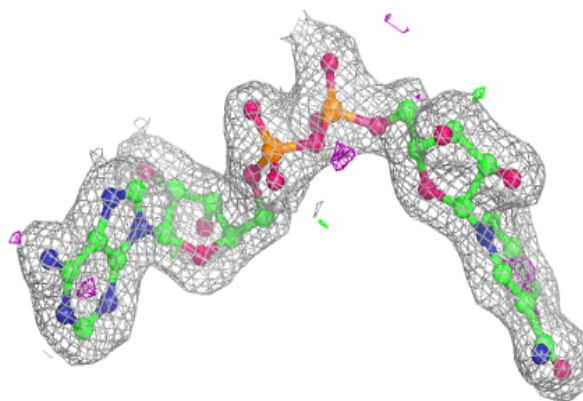
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	AE3	B	1501	9/9	0.86	0.17	37,37,38,38	0
5	PG4	C	1502	12/13	0.89	0.17	26,26,28,29	0
3	0D8	C	1500	5/5	0.90	0.15	38,42,43,47	0
3	0D8	C	1499	5/5	0.91	0.16	33,33,36,40	0
5	PG4	A	1501	12/13	0.91	0.12	26,27,29,29	0
3	0D8	B	1499	5/5	0.92	0.15	21,21,26,26	0
3	0D8	D	1498	5/5	0.94	0.13	29,31,33,33	0
4	FMT	A	1500	3/3	0.95	0.13	19,19,20,21	0
2	NAD	D	1497	44/44	0.96	0.09	14,16,18,18	0
2	NAD	C	1498	44/44	0.96	0.09	15,18,20,21	0
4	FMT	D	1499	3/3	0.96	0.10	20,20,20,21	0
3	0D8	A	1499	5/5	0.97	0.11	21,21,26,27	0
2	NAD	A	1498	44/44	0.97	0.08	13,16,18,20	0
2	NAD	B	1498	44/44	0.97	0.08	16,18,19,22	0
4	FMT	C	1501	3/3	0.97	0.09	22,22,22,24	0
6	K	A	1502	1/1	0.98	0.08	17,17,17,17	1
6	K	C	1503	1/1	0.98	0.06	26,26,26,26	1
4	FMT	B	1500	3/3	0.98	0.08	23,23,23,24	0
6	K	D	1500	1/1	0.99	0.06	20,20,20,20	1
6	K	B	1502	1/1	0.99	0.05	20,20,20,20	1

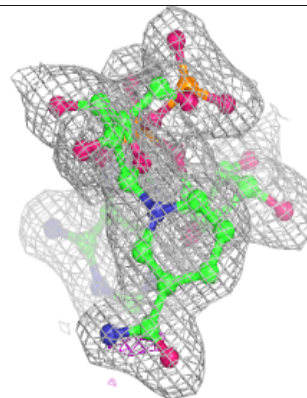
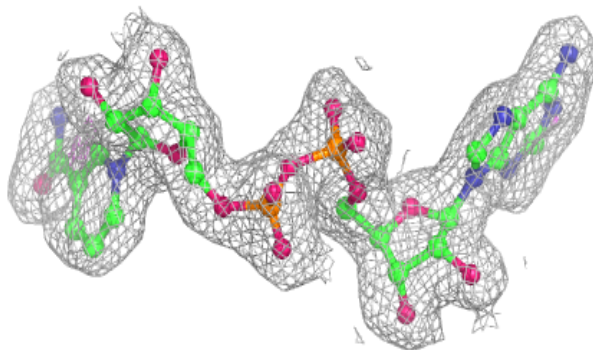
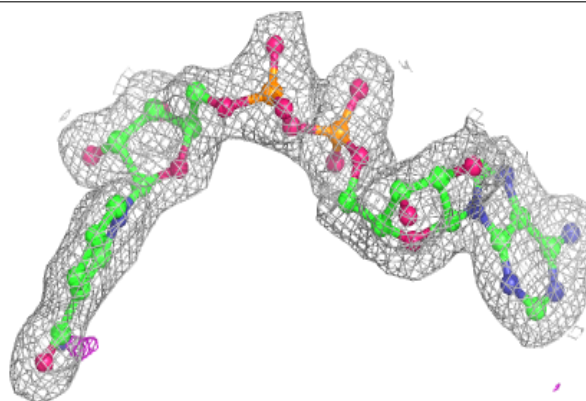
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD D 1497:**

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

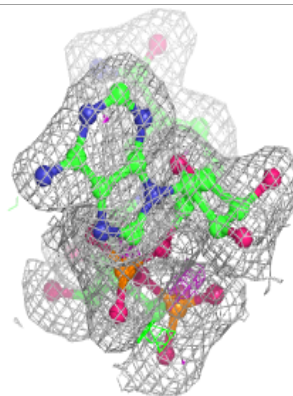
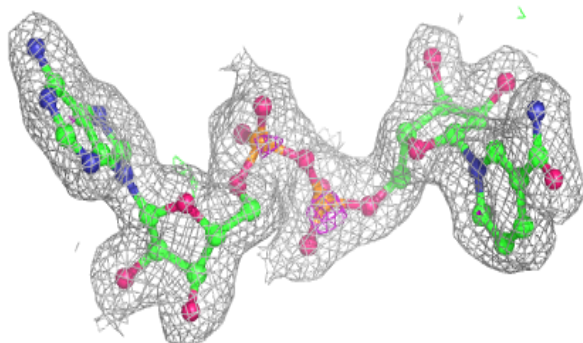
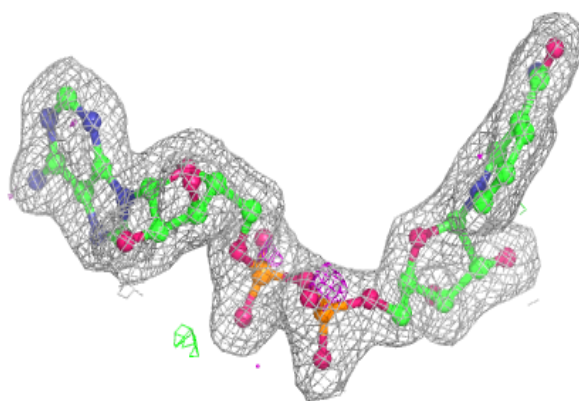
**Electron density around NAD C 1498:**

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

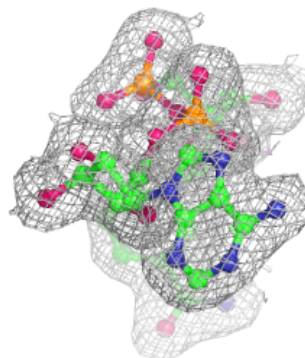
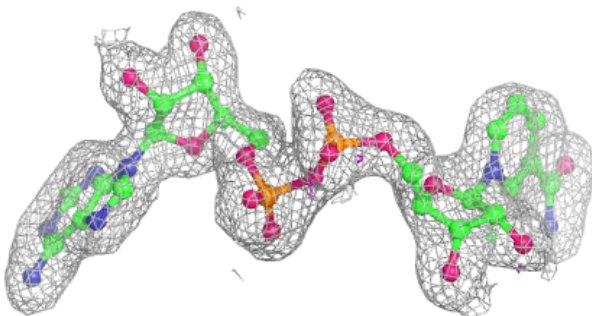
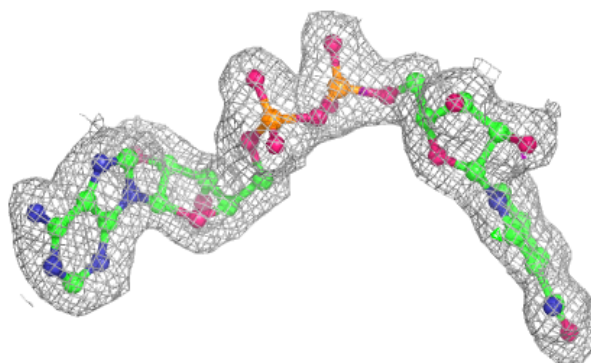


**Electron density around NAD A 1498:**

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

**Electron density around NAD B 1498:**

$2mF_o-DF_c$  (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.