



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 06:56 AM EDT

PDB ID : 6UFP  
Title : Structure of proline utilization A with the FAD covalently modified by L-thiazolidine-2-carboxylate and three cysteines (Cys46, Cys470, Cys638) modified to S,S-(2-HYDROXYETHYL)THIOCYSTEINE  
Authors : Campbell, A.C.; Tanner, J.J.  
Deposited on : 2019-09-24  
Resolution : 1.74 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

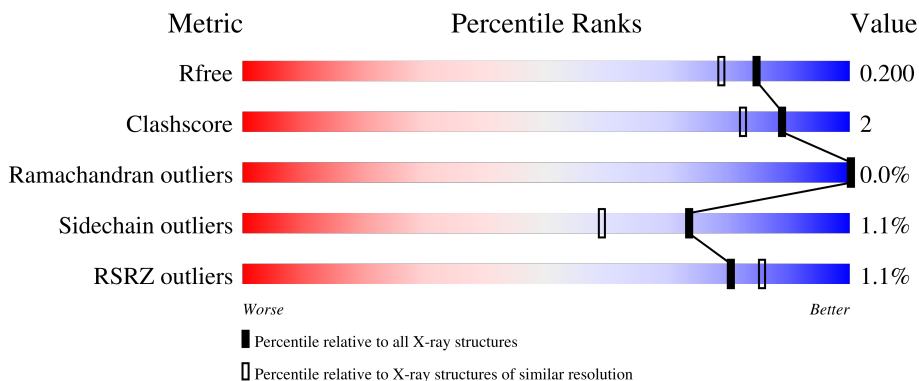
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	1235	
2	B	1235	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19186 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 Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1197	8864	5577	1585	1665	37	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3

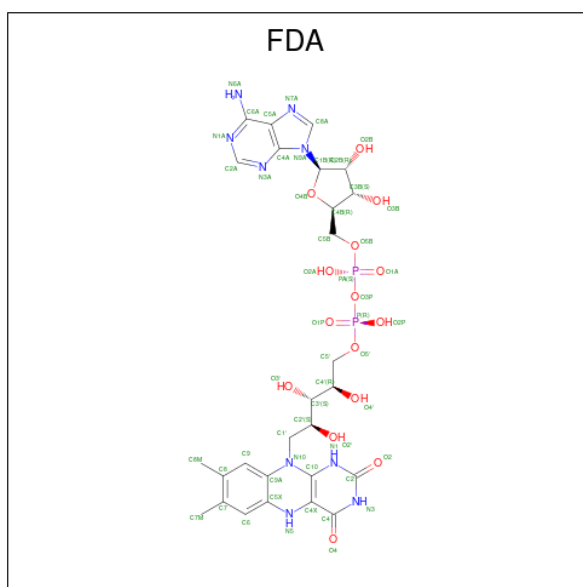
- Molecule 2 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1197	8852	5569	1594	1654	35	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

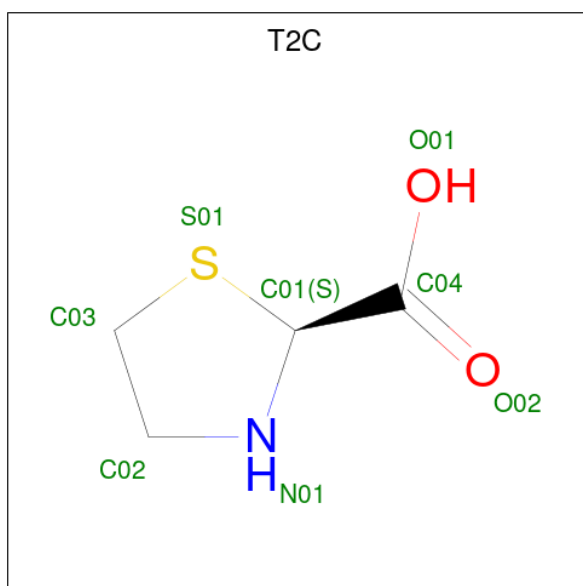
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0

- Molecule 4 is (2S)-1,3-thiazolidine-2-carboxylic acid (three-letter code: T2C) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



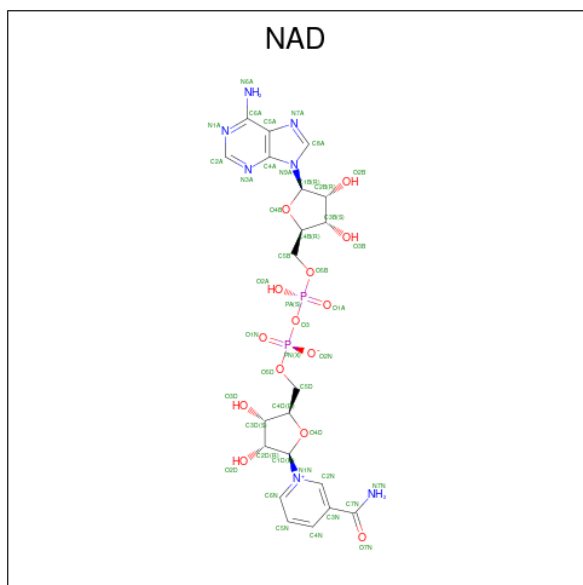
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	8	4	1	2	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	8	4	1	2	1	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	44	21	7	14	2	0	0
5	B	1	35	15	5	13	2	0	0

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



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

- Molecule 7 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



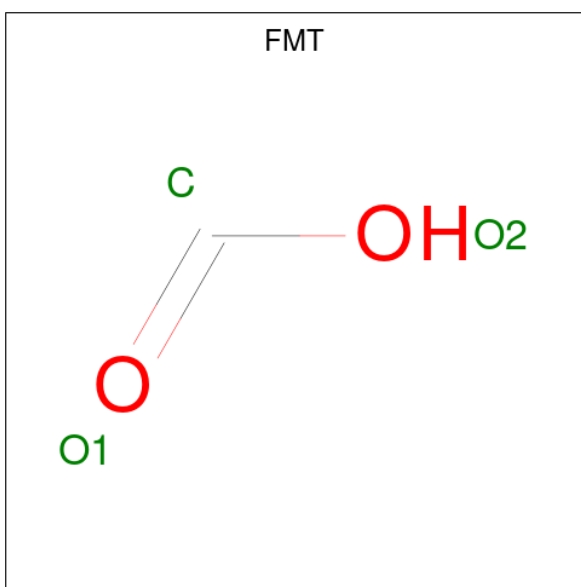
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0

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

- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

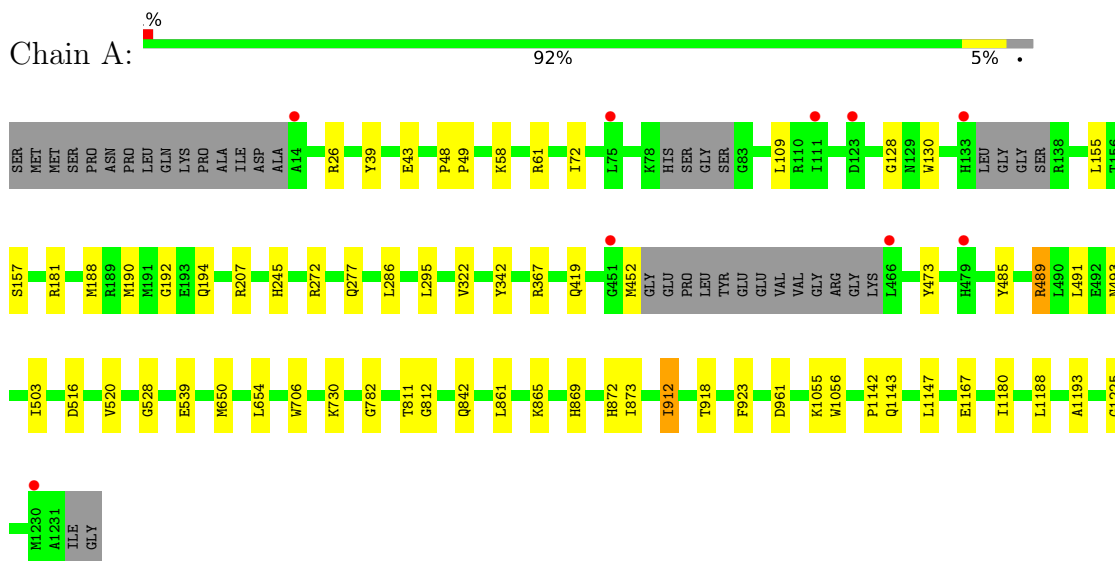
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	597	Total O 597 597	0	0
9	B	622	Total O 622 622	0	0

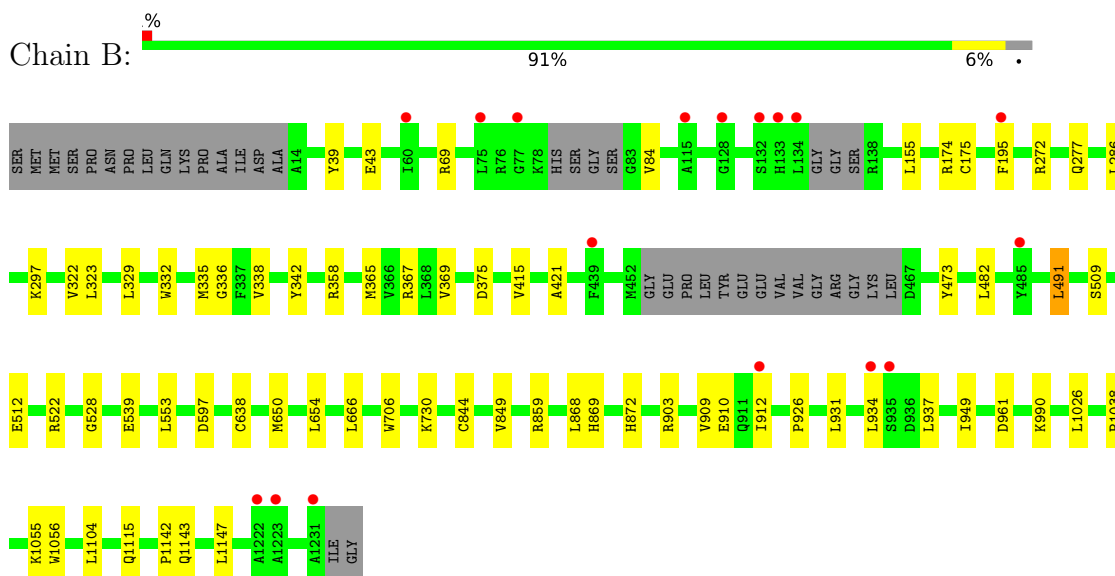
### 3 Residue-property plots [i](#)

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: Bifunctional protein PutA



- Molecule 2: Bifunctional protein PutA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.42Å 102.11Å 126.69Å 90.00° 106.46° 90.00°	Depositor
Resolution (Å)	121.50 – 1.74 121.50 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.8 (121.50-1.74) 98.8 (121.50-1.74)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 1.74Å)	Xtrriage
Refinement program	PHENIX dev_3120	Depositor
R, $R_{free}$	0.168 , 0.200 0.168 , 0.200	Depositor DCC
$R_{free}$ test set	12306 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.2	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	0.97	EDS
Total number of atoms	19186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: SO4, FDA, NAD, CME, PEG, T2C, FMT

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	0.33	0/9012	0.52	0/12271
2	B	0.34	0/8988	0.53	1/12236 (0.0%)
All	All	0.34	0/18000	0.52	1/24507 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	174	ARG	NE-CZ-NH1	5.06	122.83	120.30

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	8864	0	8849	36	0
2	B	8852	0	8853	35	0
3	A	53	0	32	1	0
3	B	53	0	32	1	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	44	0	25	1	0
5	B	35	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	7	0	10	0	0
6	B	7	0	10	0	0
7	A	20	0	0	0	0
7	B	10	0	0	0	0
8	A	3	0	1	0	0
8	B	3	0	1	0	0
9	A	597	0	0	1	0
9	B	622	0	0	3	0
All	All	19186	0	17831	69	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 (69) 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)
5:B:1303:NAD:C1D	5:B:1303:NAD:O4D	1.63	1.21
2:B:155:LEU:HD22	2:B:491:LEU:HD11	1.73	0.70
2:B:706:TRP:NE1	5:B:1303:NAD:O1N	2.27	0.67
1:A:539:GLU:OE2	9:A:1401:HOH:O	2.11	0.67
2:B:539:GLU:OE1	9:B:1401:HOH:O	2.14	0.66
1:A:1055:LYS:NZ	2:B:961:ASP:OD2	2.27	0.65
1:A:155:LEU:HD22	1:A:491:LEU:HD21	1.80	0.63
1:A:26:ARG:HH22	1:A:322:VAL:HG23	1.63	0.63
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.83	0.60
2:B:849:VAL:HG11	2:B:934:LEU:HD13	1.84	0.59
2:B:286:LEU:HD21	2:B:322:VAL:HG11	1.85	0.58
1:A:869:HIS:ND1	1:A:912:ILE:HG22	2.19	0.57
2:B:297:LYS:HD2	2:B:329:LEU:HA	1.85	0.57
1:A:706:TRP:HH2	1:A:842:GLN:CD	2.07	0.57
2:B:195:PHE:HB3	2:B:482:LEU:HD11	1.86	0.57
1:A:192:GLY:O	1:A:207:ARG:NH1	2.40	0.55
2:B:358:ARG:HG2	2:B:415:VAL:HG11	1.91	0.52
2:B:650:MET:O	2:B:654:LEU:HG	2.09	0.52
1:A:473:TYR:HB2	3:A:1301:FDA:HM72	1.91	0.52
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.47	0.50
2:B:868:LEU:HG	2:B:912:ILE:HD13	1.95	0.49
2:B:869:HIS:CD2	2:B:912:ILE:HG22	2.48	0.49
1:A:58:LYS:HD3	1:A:61:ARG:NH1	2.28	0.49
2:B:1056:TRP:CD1	2:B:1142:PRO:HD3	2.48	0.49
1:A:491:LEU:HD13	1:A:1225:GLY:HA3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:MET:HG2	1:A:493:ASN:HD21	1.78	0.48
1:A:1143:GLN:O	1:A:1147:LEU:HG	2.13	0.48
1:A:961:ASP:OD2	2:B:1055:LYS:NZ	2.39	0.48
2:B:1026:LEU:HD23	2:B:1038:PRO:HG2	1.96	0.47
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	1.95	0.47
2:B:369:VAL:HG12	2:B:421:ALA:HB3	1.96	0.46
1:A:245:HIS:CE1	1:A:295:LEU:HD11	2.50	0.46
1:A:873:ILE:HD11	1:A:912:ILE:HD11	1.96	0.46
1:A:485:TYR:O	1:A:489:ARG:HG2	2.16	0.46
2:B:323:LEU:HD13	2:B:335:MET:HE3	1.97	0.46
2:B:1143:GLN:O	2:B:1147:LEU:HG	2.16	0.45
1:A:190:MET:HA	1:A:194:GLN:HB2	1.98	0.45
1:A:861:LEU:HD22	1:A:865:LYS:HE3	1.98	0.45
1:A:918:THR:HB	1:A:923:PHE:CD1	2.52	0.45
2:B:868:LEU:HD11	2:B:926:PRO:HB2	1.99	0.45
2:B:473:TYR:HB2	3:B:1301:FDA:HM72	1.99	0.44
2:B:937:LEU:HD23	2:B:937:LEU:HA	1.88	0.44
2:B:990:LYS:HE2	2:B:990:LYS:HA	1.99	0.44
2:B:175:CYS:SG	9:B:1987:HOH:O	2.61	0.44
1:A:43:GLU:HB3	1:A:528:GLY:O	2.17	0.44
2:B:910:GLU:HB2	9:B:1811:HOH:O	2.18	0.44
2:B:931:LEU:HB2	2:B:949:ILE:HG22	2.00	0.43
2:B:297:LYS:HG3	2:B:332:TRP:HB2	2.00	0.43
2:B:903:ARG:HG3	2:B:909:VAL:HG21	1.99	0.43
2:B:43:GLU:HB3	2:B:528:GLY:O	2.18	0.43
2:B:553:LEU:HD12	2:B:666:LEU:HD13	2.01	0.43
1:A:72:ILE:HG23	1:A:503:ILE:HD11	2.00	0.42
1:A:109:LEU:HD21	1:A:188:MET:HE2	2.02	0.42
1:A:812:GLY:HA2	5:A:1303:NAD:O2D	2.20	0.42
2:B:1104:LEU:HG	2:B:1115:GLN:HB3	2.01	0.42
1:A:782:GLY:O	1:A:811:THR:HA	2.20	0.42
1:A:491:LEU:CD1	1:A:1225:GLY:HA3	2.50	0.42
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.02	0.41
1:A:516:ASP:O	1:A:520:VAL:HG23	2.21	0.41
1:A:1167:GLU:HA	1:A:1193:ALA:O	2.20	0.41
2:B:272:ARG:HB3	2:B:277:GLN:HG3	2.03	0.41
1:A:272:ARG:HB3	1:A:277:GLN:HG3	2.02	0.41
1:A:1147:LEU:HD22	2:B:1147:LEU:HD13	2.03	0.41
1:A:128:GLY:O	1:A:130:TRP:N	2.52	0.41
1:A:650:MET:O	1:A:654:LEU:HG	2.21	0.41
2:B:338:VAL:HG22	2:B:367:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:509:SER:OG	2:B:512:GLU:HG3	2.21	0.40
2:B:336:GLY:HA2	2:B:365:MET:O	2.22	0.40
1:A:48:PRO:HB2	1:A:49:PRO:HD3	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	1192/1235 (96%)	1172 (98%)	20 (2%)	0	100 100
2	B	1191/1235 (96%)	1168 (98%)	22 (2%)	1 (0%)	51 33
All	All	2383/2470 (96%)	2340 (98%)	42 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	597	ASP

### 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	885/949 (93%)	877 (99%)	8 (1%)	78 67
2	B	879/948 (93%)	868 (99%)	11 (1%)	69 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1764/1897 (93%)	1745 (99%)	19 (1%)	73 59

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	157	SER
1	A	181	ARG
1	A	342	TYR
1	A	489	ARG
1	A	730	LYS
1	A	872	HIS
1	A	912	ILE
2	B	39	TYR
2	B	69	ARG
2	B	84	VAL
2	B	342	TYR
2	B	375	ASP
2	B	491	LEU
2	B	522	ARG
2	B	730	LYS
2	B	844	CYS
2	B	859	ARG
2	B	872	HIS

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

Mol	Chain	Res	Type
1	A	493	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	CME	B	470	2	8,9,10	1.06	0	5,9,11	0.66	0
1	CME	A	470	1	8,9,10	1.01	0	5,9,11	0.58	0
2	CME	B	638	2	8,9,10	0.83	0	5,9,11	2.11	1 (20%)
2	CME	B	46	2	8,9,10	0.93	0	5,9,11	0.76	0
1	CME	A	46	1	8,9,10	0.98	0	5,9,11	0.62	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
2	CME	B	470	2	-	2/5/8/10	-
1	CME	A	470	1	-	1/5/8/10	-
2	CME	B	638	2	-	2/5/8/10	-
2	CME	B	46	2	-	1/5/8/10	-
1	CME	A	46	1	-	1/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	638	CME	CB-SG-SD	4.40	115.22	103.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	470	CME	SD-CE-CZ-OH
2	B	470	CME	SD-CE-CZ-OH
2	B	638	CME	CE-SD-SG-CB
1	A	46	CME	CZ-CE-SD-SG
2	B	46	CME	CZ-CE-SD-SG
2	B	470	CME	CZ-CE-SD-SG
2	B	638	CME	CA-CB-SG-SD

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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
7	SO4	B	1305	-	4,4,4	0.32	0	6,6,6	0.36	0
6	PEG	A	1304	-	6,6,6	0.49	0	5,5,5	0.24	0
7	SO4	A	1307	-	4,4,4	0.14	0	6,6,6	0.10	0
7	SO4	A	1305	-	4,4,4	0.14	0	6,6,6	0.28	0
5	NAD	B	1303	-	33,38,48	5.21	15 (45%)	37,58,73	1.71	6 (16%)
7	SO4	A	1306	-	4,4,4	0.13	0	6,6,6	0.08	0
8	FMT	B	1307	-	2,2,2	0.70	0	1,1,1	0.26	0
4	T2C	B	1302	3	7,8,8	0.97	0	6,10,10	1.96	3 (50%)
4	T2C	A	1302	3	7,8,8	1.00	0	6,10,10	2.17	3 (50%)
5	NAD	A	1303	-	42,48,48	5.39	18 (42%)	50,73,73	1.67	8 (16%)
7	SO4	A	1308	-	4,4,4	0.15	0	6,6,6	0.14	0
3	FDA	A	1301	4	52,58,58	2.43	19 (36%)	60,89,89	1.51	9 (15%)
7	SO4	B	1306	-	4,4,4	0.14	0	6,6,6	0.16	0
8	FMT	A	1309	-	2,2,2	0.65	0	1,1,1	0.08	0
6	PEG	B	1304	-	6,6,6	0.49	0	5,5,5	0.21	0
3	FDA	B	1301	4	52,58,58	2.54	17 (32%)	60,89,89	1.53	7 (11%)

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. '2' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	1304	-	-	1/4/4/4	-
5	NAD	B	1303	-	-	4/18/51/62	0/4/4/5
4	T2C	B	1302	3	-	0/3/11/11	0/1/1/1
4	T2C	A	1302	3	-	0/3/11/11	0/1/1/1
5	NAD	A	1303	-	-	3/26/62/62	0/5/5/5
3	FDA	A	1301	4	-	6/30/50/50	0/6/6/6
6	PEG	B	1304	-	-	0/4/4/4	-
3	FDA	B	1301	4	-	6/30/50/50	0/6/6/6

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1303	NAD	C2D-C1D	-16.36	1.28	1.53
5	A	1303	NAD	O4D-C1D	15.76	1.63	1.41
5	A	1303	NAD	O4B-C1B	15.75	1.63	1.41
5	B	1303	NAD	O4B-C1B	15.42	1.62	1.41
5	B	1303	NAD	C2B-C1B	-15.21	1.30	1.53
5	A	1303	NAD	C2B-C1B	-15.19	1.30	1.53
5	B	1303	NAD	C1D-C2D	-13.16	1.29	1.51
5	B	1303	NAD	O4D-C1D	8.94	1.63	1.43
3	B	1301	FDA	O4-C4	7.41	1.37	1.23
5	A	1303	NAD	C7N-N7N	6.80	1.45	1.33
5	B	1303	NAD	O4D-C4D	-6.66	1.33	1.44
3	A	1301	FDA	O4-C4	6.49	1.35	1.23
5	A	1303	NAD	O4B-C4B	-6.32	1.30	1.45
5	B	1303	NAD	O4B-C4B	-6.27	1.31	1.45
3	A	1301	FDA	C6-C5X	6.25	1.49	1.39
3	B	1301	FDA	O2-C2	6.22	1.36	1.23
3	B	1301	FDA	C6-C5X	6.13	1.49	1.39
3	A	1301	FDA	O2-C2	6.02	1.36	1.23
5	A	1303	NAD	O4D-C4D	-5.13	1.33	1.45
3	B	1301	FDA	C9-C9A	4.96	1.47	1.39
3	A	1301	FDA	C9-C9A	4.95	1.47	1.39
3	B	1301	FDA	C4X-N5	4.35	1.45	1.35
3	A	1301	FDA	C4X-N5	4.30	1.45	1.35
3	B	1301	FDA	C5X-C9A	-3.71	1.36	1.40
3	B	1301	FDA	C10-N1	3.63	1.43	1.37
3	B	1301	FDA	C4X-C4	3.57	1.51	1.42
3	B	1301	FDA	C2-N1	3.55	1.43	1.37
3	B	1301	FDA	C5X-N5	3.55	1.46	1.39
5	B	1303	NAD	C6A-N6A	3.53	1.46	1.34
5	A	1303	NAD	C6A-N6A	3.52	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	FDA	C10-N1	3.48	1.43	1.37
3	A	1301	FDA	C5X-C9A	-3.42	1.36	1.40
5	A	1303	NAD	O3D-C3D	-3.36	1.35	1.43
3	A	1301	FDA	C2B-C1B	-3.33	1.48	1.53
3	A	1301	FDA	C2-N1	3.29	1.43	1.37
3	B	1301	FDA	C2A-N3A	3.29	1.37	1.32
3	B	1301	FDA	C2B-C1B	-3.27	1.48	1.53
5	B	1303	NAD	O3D-C3D	-3.18	1.35	1.43
5	B	1303	NAD	O2D-C2D	3.15	1.50	1.43
5	A	1303	NAD	O2B-C2B	3.14	1.50	1.43
3	A	1301	FDA	C5X-N5	3.13	1.45	1.39
5	B	1303	NAD	O2B-C2B	3.08	1.50	1.43
5	A	1303	NAD	O2D-C2D	2.94	1.49	1.43
3	A	1301	FDA	C2A-N3A	2.88	1.36	1.32
5	A	1303	NAD	C5A-C4A	-2.84	1.33	1.40
3	B	1301	FDA	C10-N10	2.83	1.43	1.38
5	A	1303	NAD	O7N-C7N	-2.79	1.18	1.24
5	B	1303	NAD	C5A-C4A	-2.76	1.33	1.40
3	A	1301	FDA	C4X-C4	2.76	1.49	1.42
5	A	1303	NAD	C3N-C7N	2.71	1.54	1.50
3	A	1301	FDA	C6A-N6A	2.66	1.43	1.34
3	B	1301	FDA	C6A-N6A	2.60	1.43	1.34
5	B	1303	NAD	O3B-C3B	-2.58	1.36	1.43
5	A	1303	NAD	C5B-C4B	2.53	1.59	1.51
3	A	1301	FDA	PA-O5B	-2.51	1.49	1.59
3	A	1301	FDA	O3B-C3B	-2.45	1.37	1.43
5	A	1303	NAD	O3B-C3B	-2.41	1.37	1.43
5	B	1303	NAD	C2D-C3D	2.39	1.57	1.53
3	A	1301	FDA	PA-O2A	-2.35	1.44	1.55
3	A	1301	FDA	C10-N10	2.33	1.42	1.38
3	B	1301	FDA	PA-O2A	-2.32	1.44	1.55
3	B	1301	FDA	C9A-N10	2.23	1.45	1.41
5	A	1303	NAD	C2A-N3A	2.22	1.35	1.32
3	B	1301	FDA	C2-N3	2.21	1.41	1.37
5	B	1303	NAD	C5B-C4B	2.19	1.58	1.51
3	A	1301	FDA	O2'-C2'	-2.15	1.38	1.43
5	B	1303	NAD	C2A-N3A	2.14	1.35	1.32
5	A	1303	NAD	C2N-N1N	2.11	1.37	1.35
3	A	1301	FDA	C9A-N10	2.00	1.44	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1303	NAD	N3A-C2A-N1A	-5.90	119.45	128.68
3	B	1301	FDA	N3A-C2A-N1A	-5.86	119.52	128.68
5	A	1303	NAD	C5A-C6A-N6A	5.72	129.04	120.35
5	A	1303	NAD	N3A-C2A-N1A	-5.29	120.41	128.68
3	A	1301	FDA	N3A-C2A-N1A	-5.28	120.42	128.68
5	B	1303	NAD	C5A-C6A-N6A	4.80	127.64	120.35
3	A	1301	FDA	C4-N3-C2	-4.24	120.24	126.34
3	B	1301	FDA	C4-N3-C2	-4.19	120.30	126.34
5	A	1303	NAD	N6A-C6A-N1A	-3.83	110.61	118.57
4	A	1302	T2C	C02-C03-S01	-3.56	100.02	106.15
5	A	1303	NAD	C3N-C7N-N7N	3.53	121.99	117.75
3	B	1301	FDA	N3-C2-N1	3.48	121.40	115.80
5	B	1303	NAD	N6A-C6A-N1A	-3.35	111.63	118.57
3	A	1301	FDA	N3-C2-N1	3.15	120.87	115.80
5	A	1303	NAD	O4D-C1D-C2D	-3.05	102.47	106.93
3	B	1301	FDA	C1B-N9A-C4A	-2.99	121.40	126.64
3	A	1301	FDA	C5X-N5-C4X	-2.92	114.11	121.02
5	B	1303	NAD	C1D-C2D-C3D	2.72	105.78	101.63
4	B	1302	T2C	C02-C03-S01	-2.67	101.55	106.15
3	A	1301	FDA	C4X-C4-N3	2.54	119.86	112.31
3	B	1301	FDA	C5X-N5-C4X	-2.53	115.03	121.02
4	B	1302	T2C	C03-C02-N01	2.47	111.18	107.23
5	B	1303	NAD	O4B-C1B-C2B	-2.43	103.37	106.93
5	A	1303	NAD	O7N-C7N-N7N	-2.41	119.15	122.58
4	B	1302	T2C	C02-N01-C01	2.39	111.08	106.19
4	A	1302	T2C	C02-N01-C01	2.38	111.08	106.19
5	B	1303	NAD	PN-O3-PA	-2.29	124.95	132.83
3	A	1301	FDA	O5'-P-O1P	2.24	117.81	109.07
4	A	1302	T2C	C03-C02-N01	2.22	110.78	107.23
3	A	1301	FDA	C1'-N10-C9A	2.21	124.19	120.51
3	B	1301	FDA	C4X-C4-N3	2.20	118.87	112.31
3	B	1301	FDA	C4A-C5A-N7A	-2.13	107.18	109.40
5	A	1303	NAD	O4B-C1B-C2B	-2.10	103.85	106.93
5	A	1303	NAD	PN-O3-PA	-2.03	125.85	132.83
3	A	1301	FDA	C1B-N9A-C4A	-2.03	123.08	126.64
3	A	1301	FDA	O4-C4-C4X	-2.02	122.61	127.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1303	NAD	C5B-O5B-PA-O1A
3	B	1301	FDA	O3'-C3'-C4'-O4'

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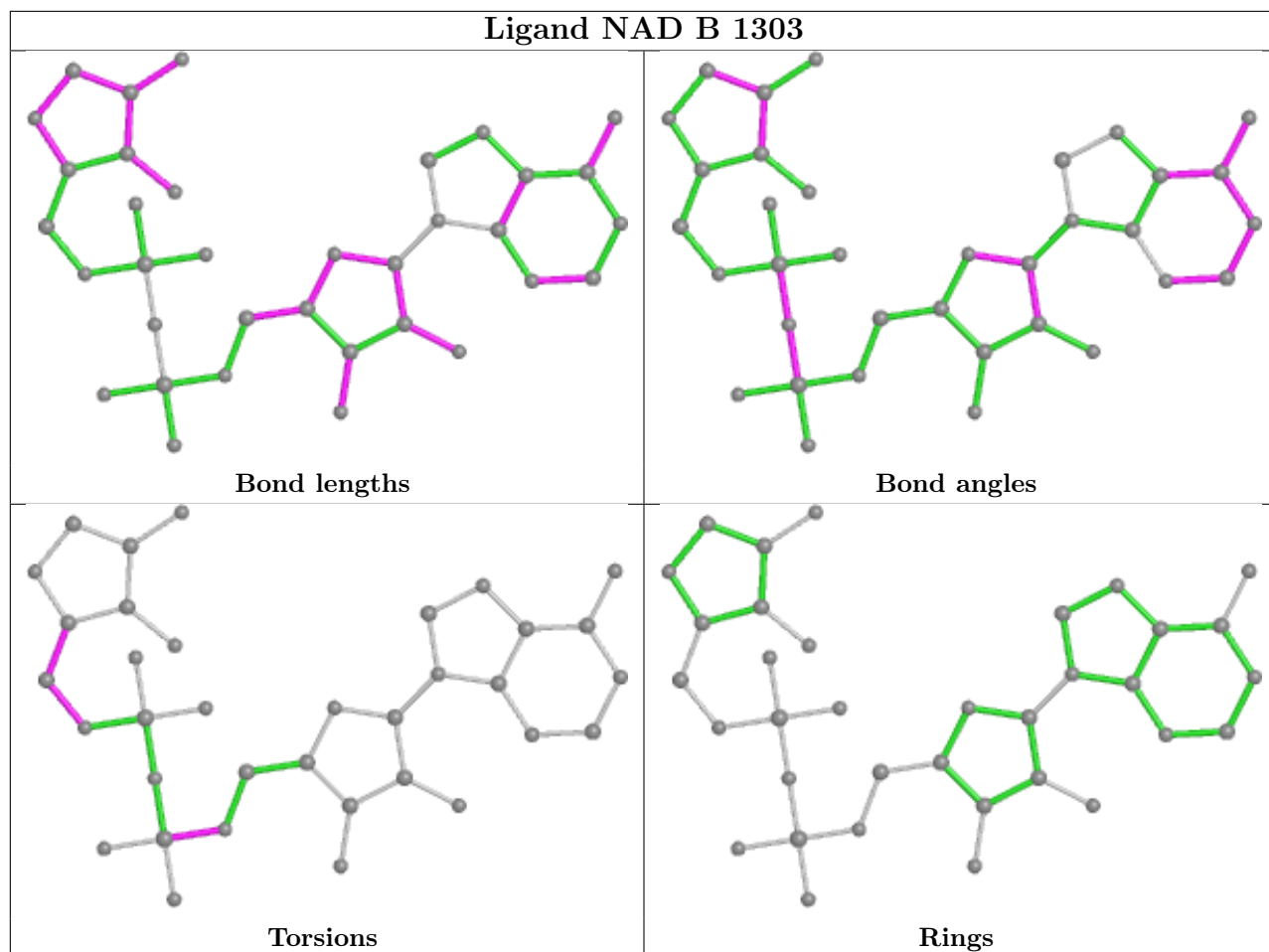
Mol	Chain	Res	Type	Atoms
3	B	1301	FDA	C2'-C3'-C4'-O4'
3	B	1301	FDA	O3'-C3'-C4'-C5'
3	B	1301	FDA	C2'-C3'-C4'-C5'
3	A	1301	FDA	O3'-C3'-C4'-C5'
3	A	1301	FDA	C2'-C3'-C4'-C5'
3	A	1301	FDA	C2'-C3'-C4'-O4'
5	A	1303	NAD	C3D-C4D-C5D-O5D
5	B	1303	NAD	C4D-C5D-O5D-PN
3	A	1301	FDA	O3'-C3'-C4'-O4'
5	B	1303	NAD	C5B-O5B-PA-O3
3	B	1301	FDA	PA-O3P-P-O2P
6	A	1304	PEG	C1-C2-O2-C3
5	A	1303	NAD	C4D-C5D-O5D-PN
5	A	1303	NAD	O4D-C4D-C5D-O5D
3	A	1301	FDA	PA-O3P-P-O1P
3	A	1301	FDA	PA-O3P-P-O2P
3	B	1301	FDA	PA-O3P-P-O1P
5	B	1303	NAD	C3D-C4D-C5D-O5D

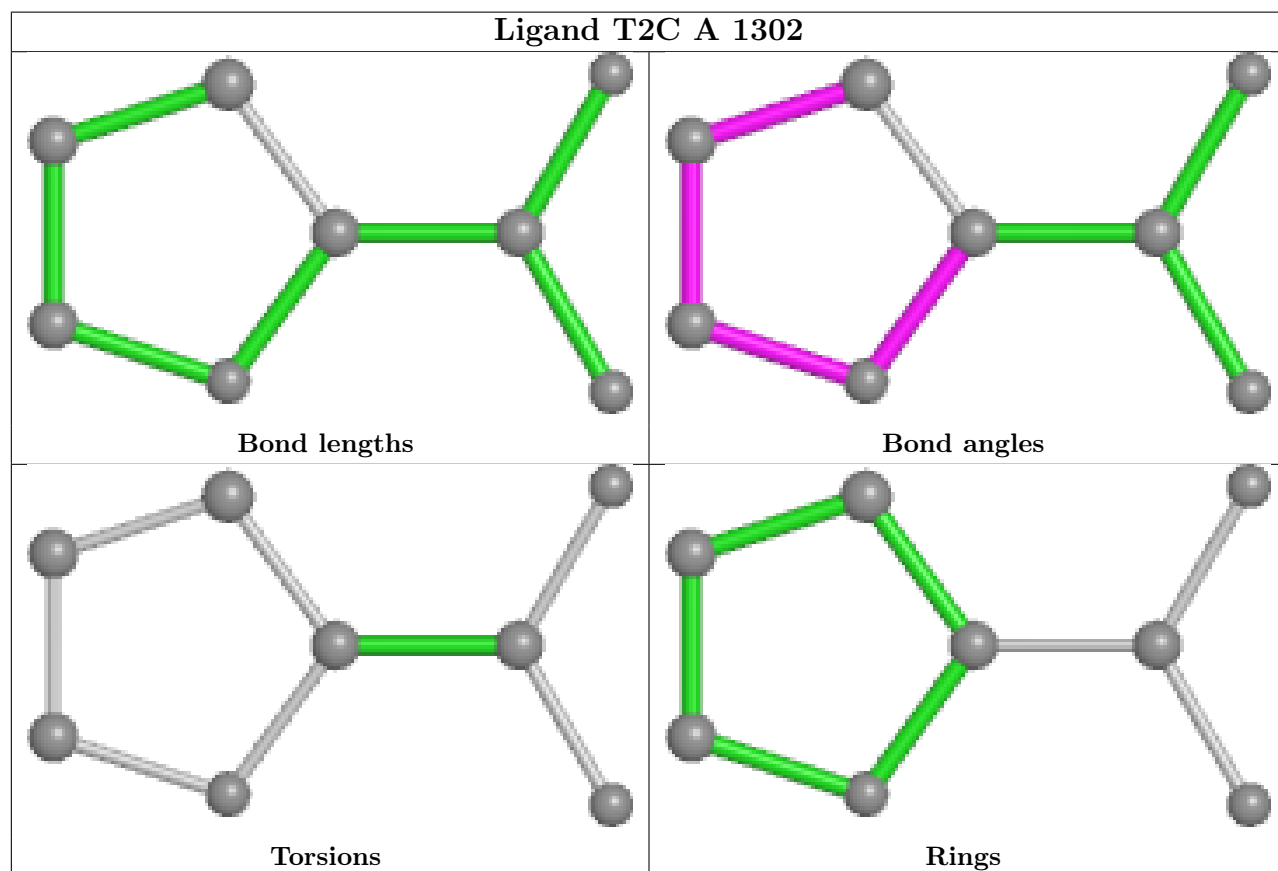
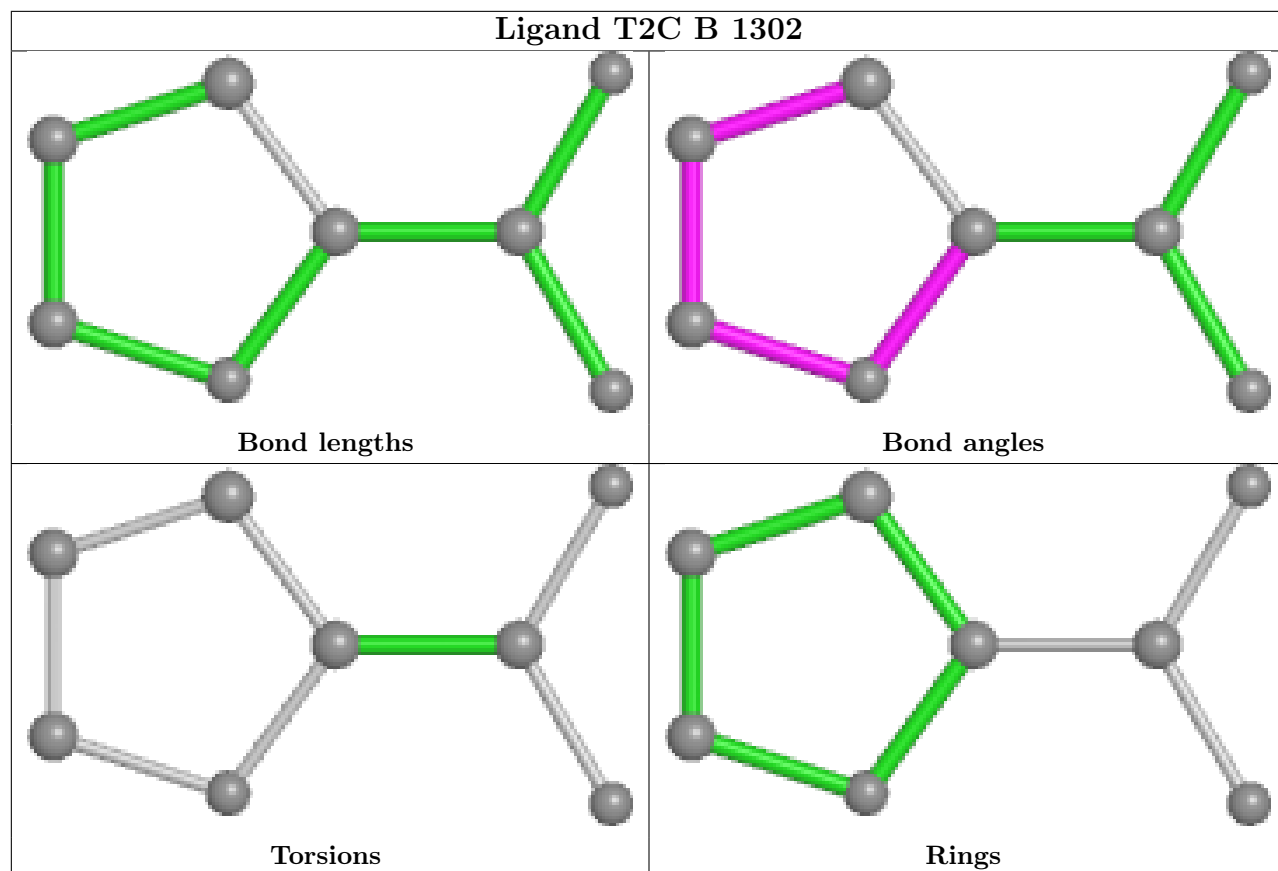
There are no ring outliers.

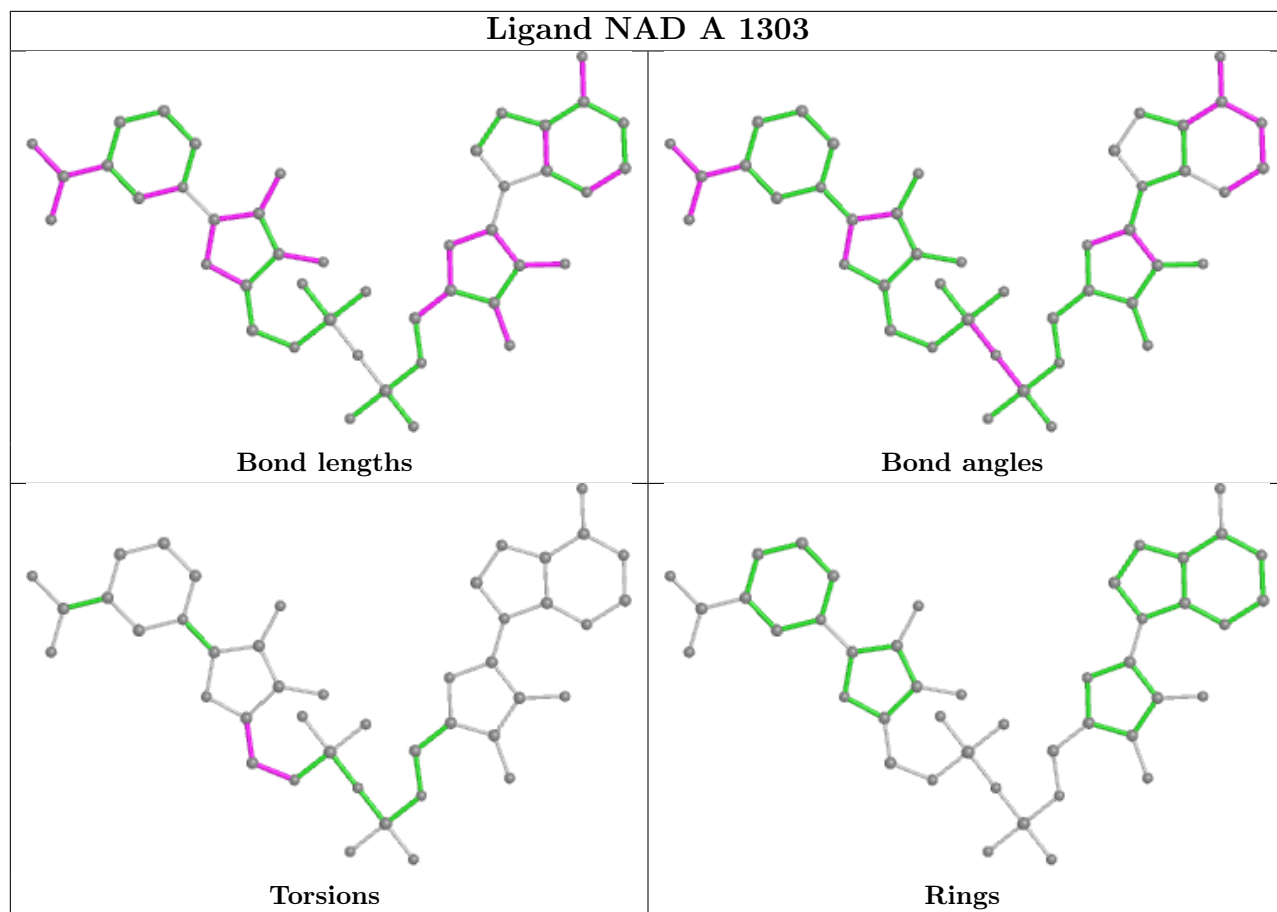
4 monomers are involved in 5 short contacts:

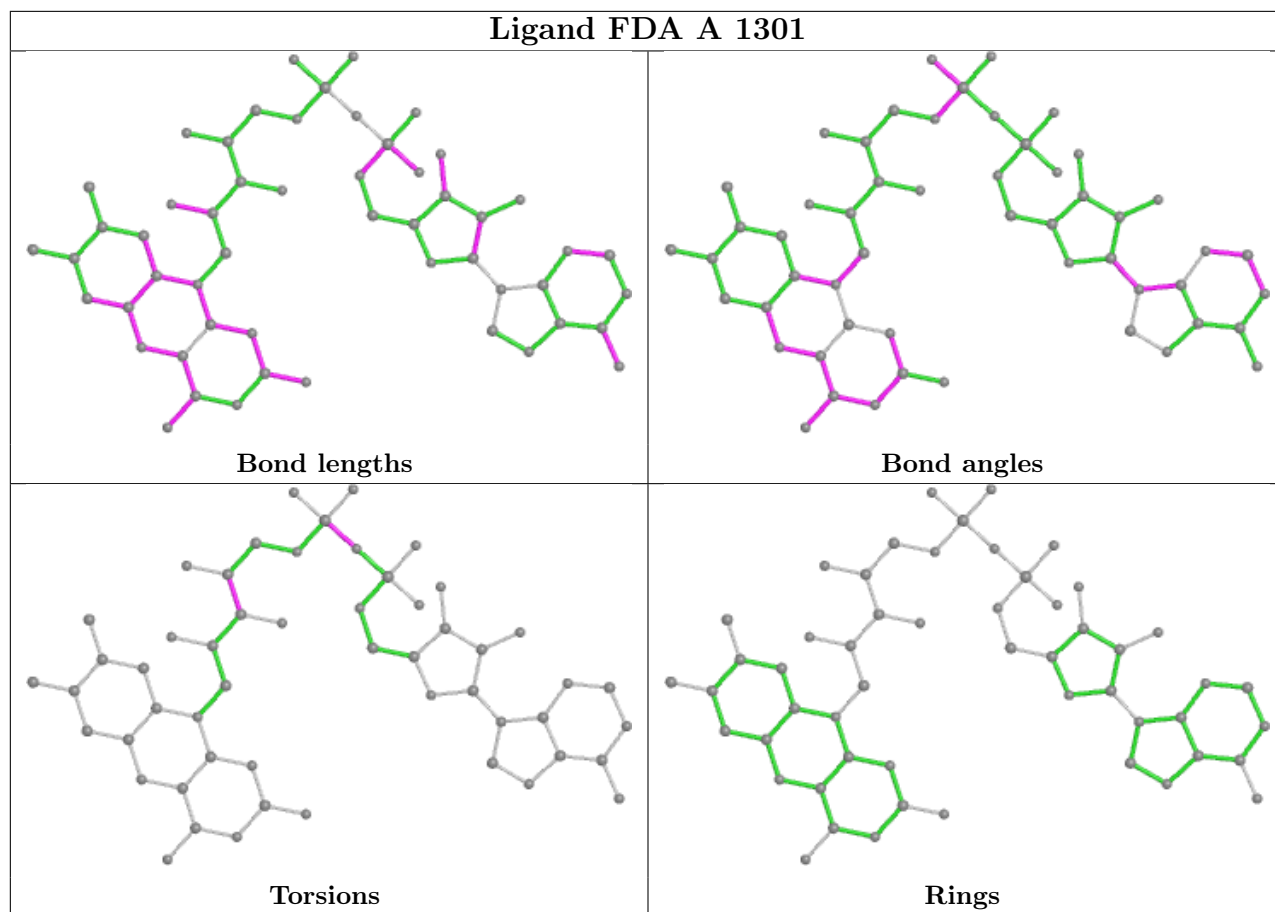
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1303	NAD	2	0
5	A	1303	NAD	1	0
3	A	1301	FDA	1	0
3	B	1301	FDA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

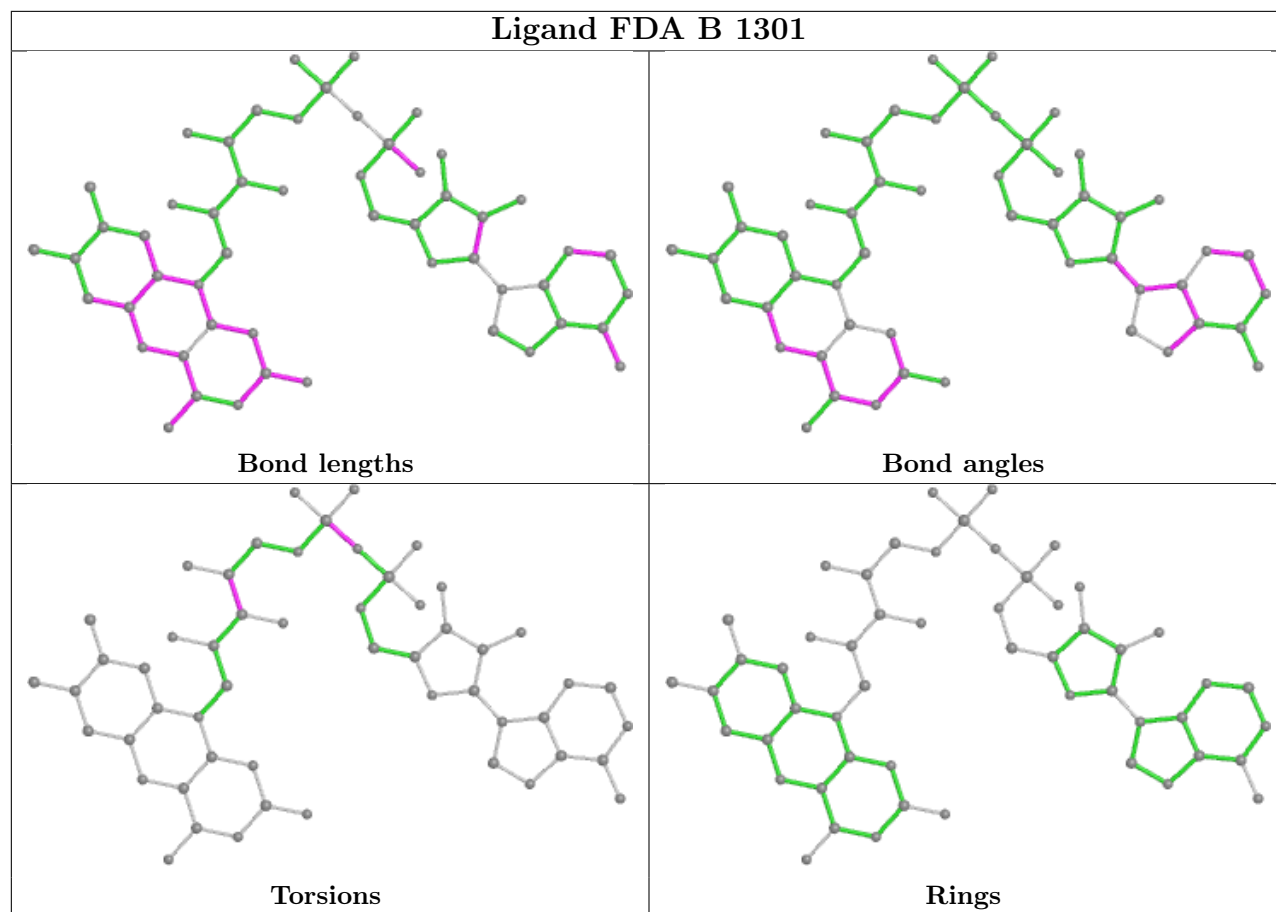












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1195/1235 (96%)	-0.41	9 (0%) 86 90	24, 37, 64, 101	0
2	B	1194/1235 (96%)	-0.33	17 (1%) 75 81	23, 36, 65, 98	1 (0%)
All	All	2389/2470 (96%)	-0.37	26 (1%) 80 85	23, 37, 64, 101	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	77	GLY	5.1
2	B	75	LEU	3.4
2	B	485	TYR	3.2
2	B	60	ILE	3.1
2	B	128	GLY	3.0
1	A	123	ASP	3.0
2	B	912	ILE	3.0
1	A	111	ILE	2.9
2	B	132	SER	2.9
1	A	14	ALA	2.8
2	B	1223	ALA	2.6
2	B	133	HIS	2.5
2	B	1222	ALA	2.5
1	A	451	GLY	2.5
1	A	1230	MET	2.5
1	A	479	HIS	2.5
1	A	75	LEU	2.4
2	B	935	SER	2.4
1	A	466	LEU	2.3
2	B	115	ALA	2.3
2	B	134	LEU	2.2
1	A	133	HIS	2.1
2	B	934	LEU	2.1
2	B	1231	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	195	PHE	2.0
2	B	439	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	CME	B	470	10/11	0.92	0.12	45,54,66,74	0
1	CME	A	470	10/11	0.94	0.08	34,40,58,63	0
2	CME	B	638	10/11	0.95	0.09	23,31,68,74	0
1	CME	A	46	10/11	0.96	0.07	39,41,55,60	0
2	CME	B	46	10/11	0.96	0.06	34,39,53,62	0

## 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.

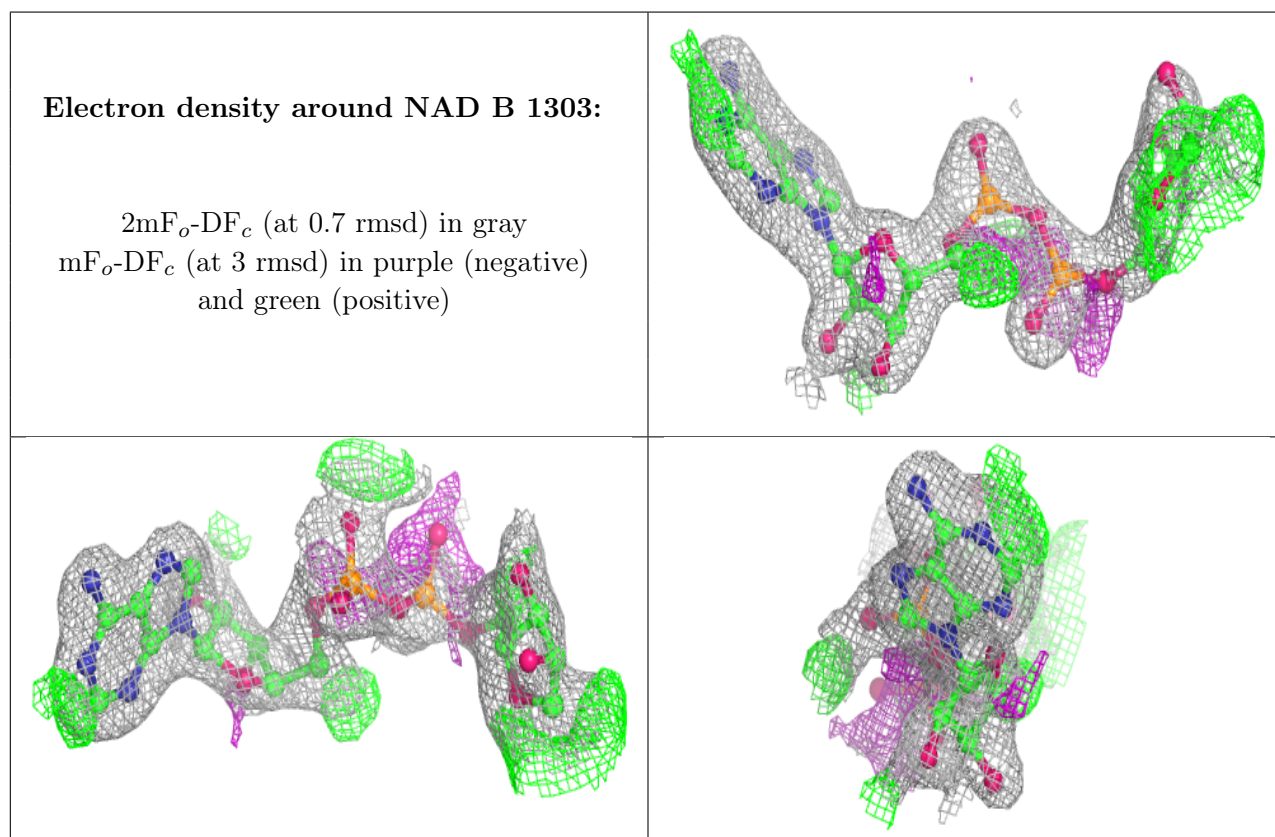
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PEG	B	1304	7/7	0.80	0.14	62,65,66,67	0
5	NAD	B	1303	35/44	0.81	0.14	32,50,74,88	35
7	SO4	A	1306	5/5	0.83	0.15	83,83,88,94	5
6	PEG	A	1304	7/7	0.86	0.13	54,61,71,73	0
5	NAD	A	1303	44/44	0.87	0.11	42,60,73,82	0
7	SO4	B	1306	5/5	0.87	0.13	76,82,84,85	5
8	FMT	A	1309	3/3	0.90	0.16	48,48,54,55	0
7	SO4	A	1307	5/5	0.91	0.10	86,91,92,100	0
3	FDA	B	1301	53/53	0.95	0.08	26,32,43,46	0
7	SO4	A	1308	5/5	0.95	0.18	63,73,84,85	0
4	T2C	A	1302	8/8	0.96	0.09	32,36,39,43	0

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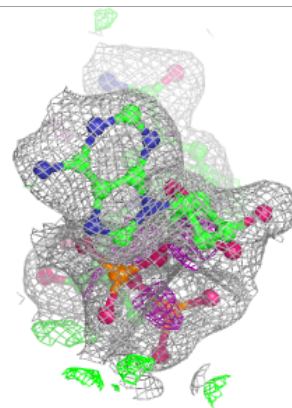
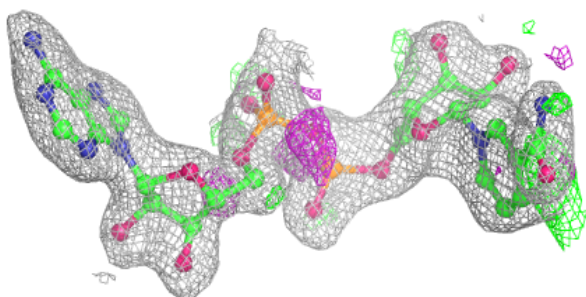
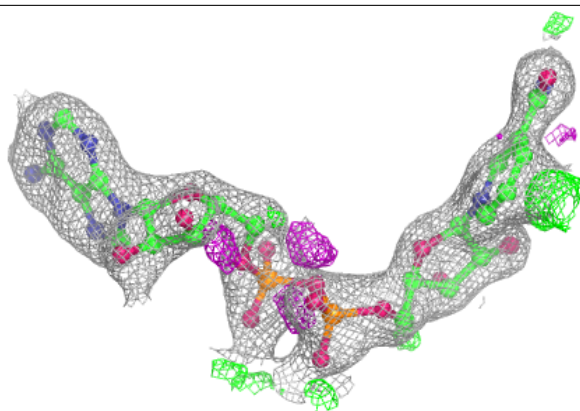
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	T2C	B	1302	8/8	0.97	0.09	32,37,40,40	0
3	FDA	A	1301	53/53	0.97	0.07	23,32,43,48	0
8	FMT	B	1307	3/3	0.97	0.11	44,44,45,49	0
7	SO4	B	1305	5/5	0.99	0.07	32,33,35,36	0
7	SO4	A	1305	5/5	0.99	0.08	32,33,34,36	0

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.

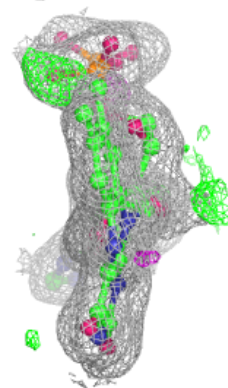
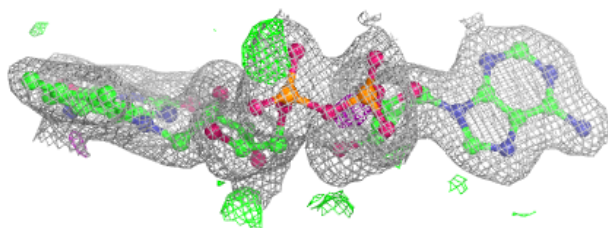
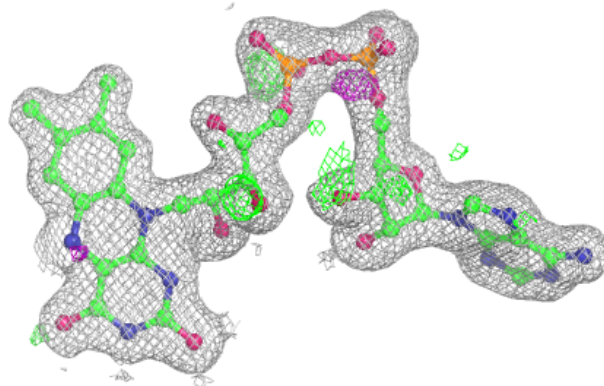


**Electron density around NAD A 1303:**

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

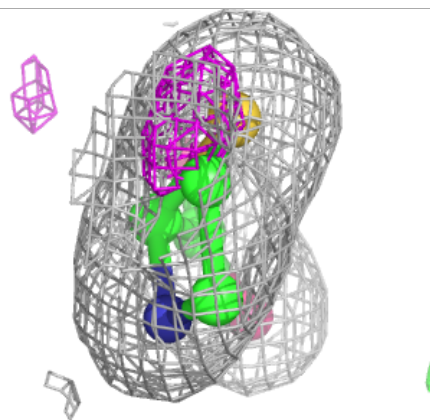
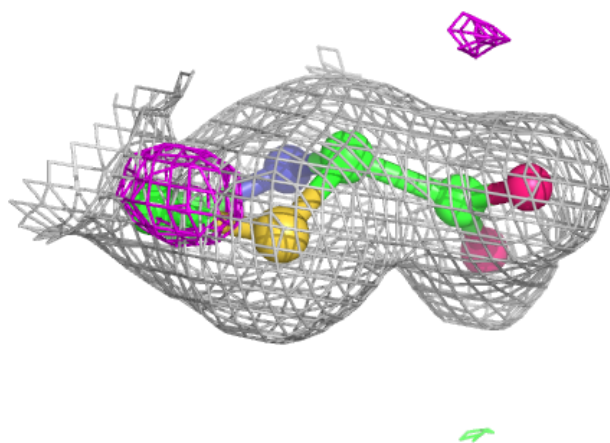
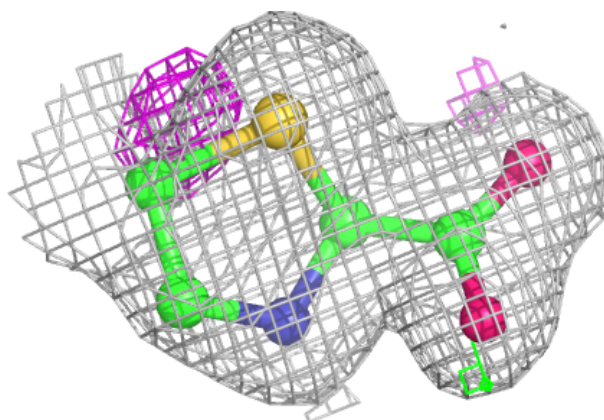
**Electron density around FDA B 1301:**

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



**Electron density around T2C A 1302:**

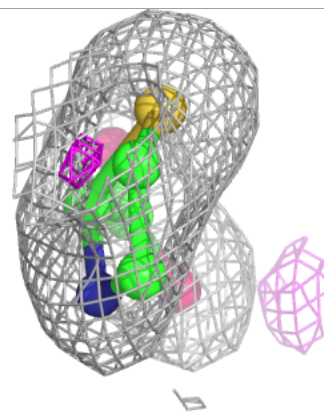
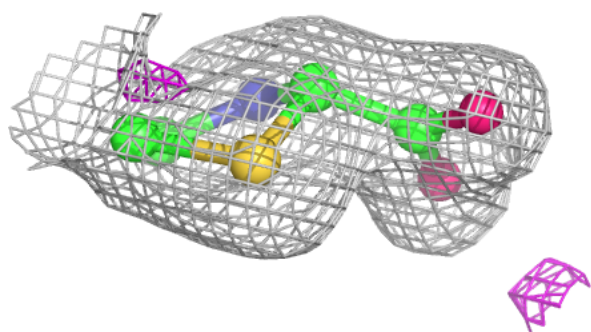
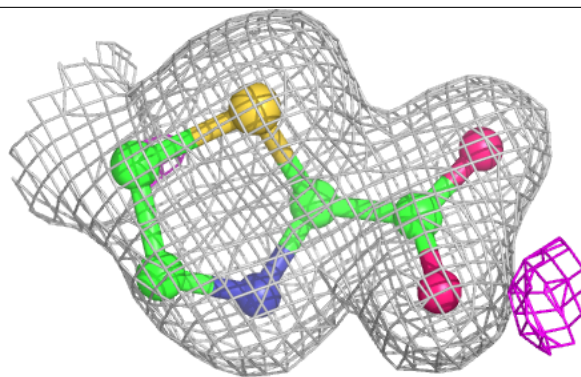
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



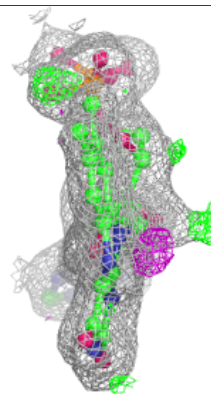
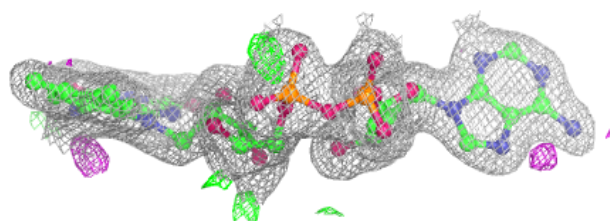
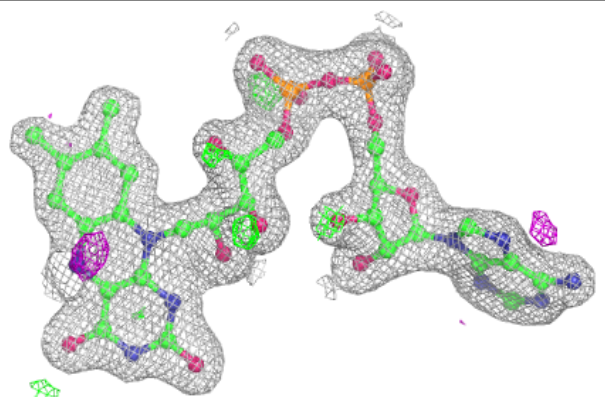


**Electron density around T2C B 1302:**

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

**Electron density around FDA A 1301:**

$2mF_o-DF_c$  (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.