



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2022 – 12:10 PM JST

PDB ID : 7WAR  
Title : SbSOMT2 in complex with pinostilbene and nicotinamide adenine dinucleotide(NAD+)  
Authors : Pow, K.C.; Hao, Q.  
Deposited on : 2021-12-14  
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>.

---

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	:	2.31.3
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)	:	2.31.3

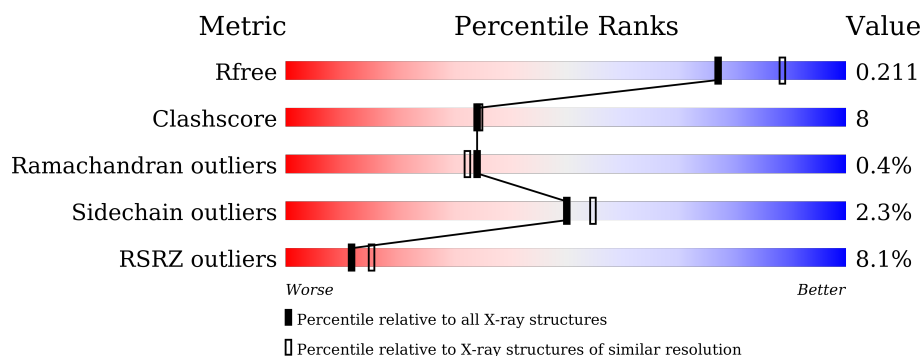
# 1 Overall quality at a glance

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	376	<div> <div>9%</div> <div>81%</div> <div>14%</div> <div>..</div> </div>
1	B	376	<div> <div>7%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAD	B	402	-	-	-	X
4	GOL	B	407	-	-	X	-
4	GOL	B	411	-	-	X	-
5	EDO	B	417	-	X	X	-

## 2 Entry composition [i](#)

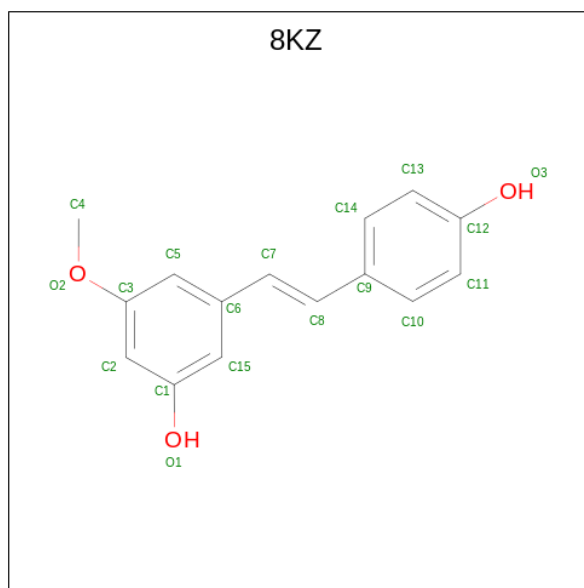
There are 9 unique types of molecules in this entry. The entry contains 6216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 stilbene O-methyltransferase.

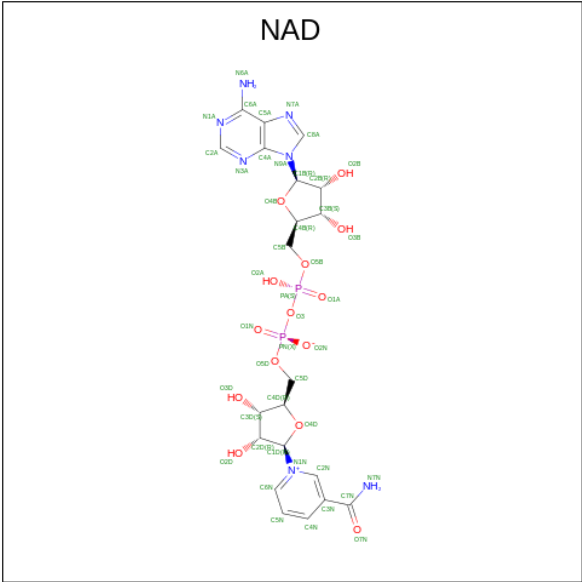
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	362	Total	C	N	O	S	0	3	0
			2830	1807	474	526	23			
1	A	363	Total	C	N	O	S	0	4	0
			2844	1813	476	532	23			

- Molecule 2 is 3-[(E)-2-(4-hydroxyphenyl)ethenyl]-5-methoxy-phenol (three-letter code: 8KZ) (formula: C<sub>15</sub>H<sub>14</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



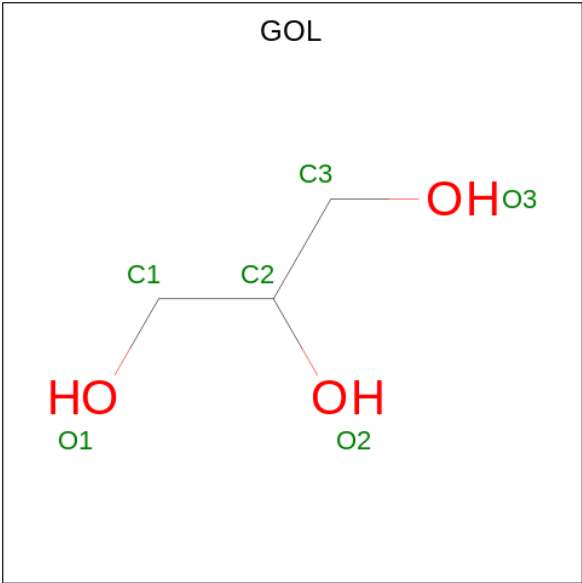
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			18	15	3		
2	A	1	Total	C	O	0	0
			18	15	3		

- Molecule 3 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
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



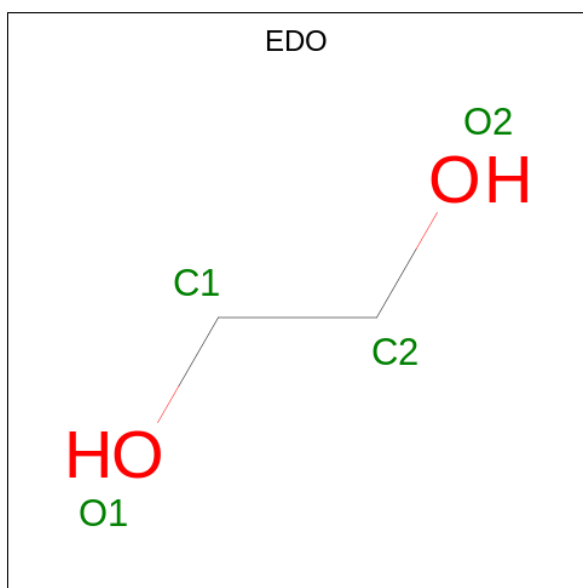
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

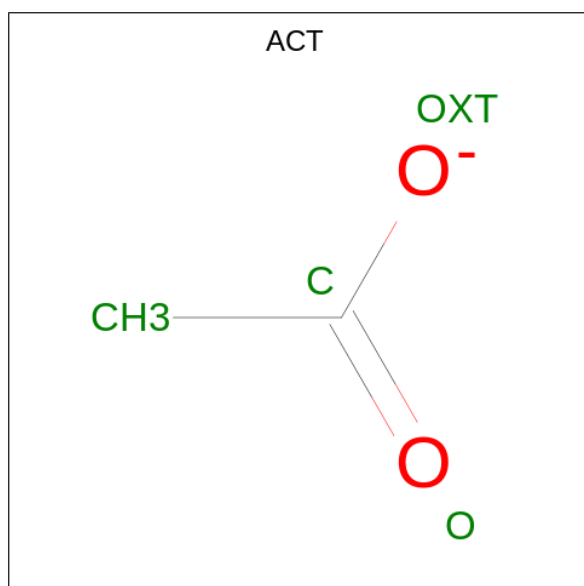
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



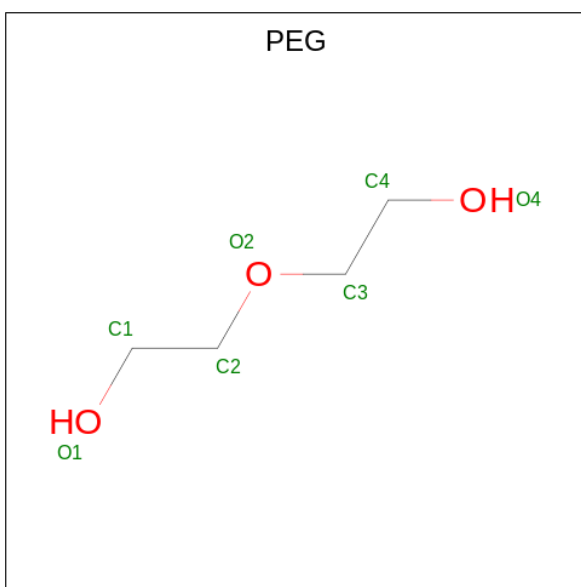
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



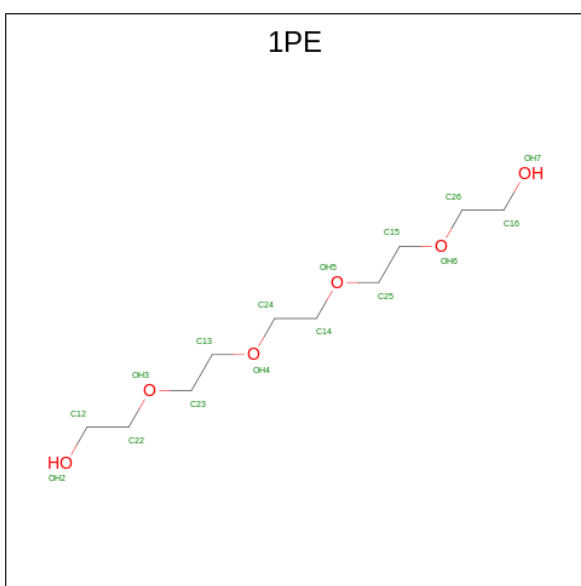
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			16	10	6		

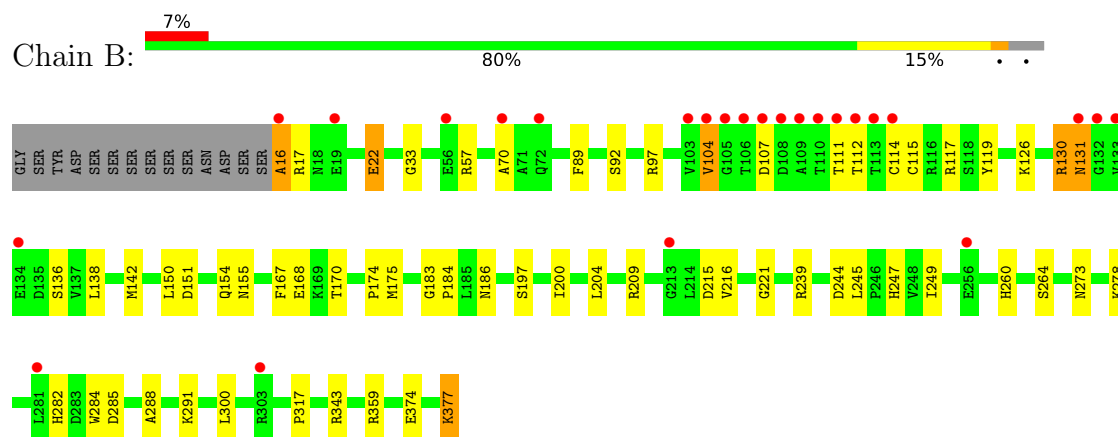
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	127	Total 127	O 127	0	0
9	A	141	Total 141	O 141	0	0

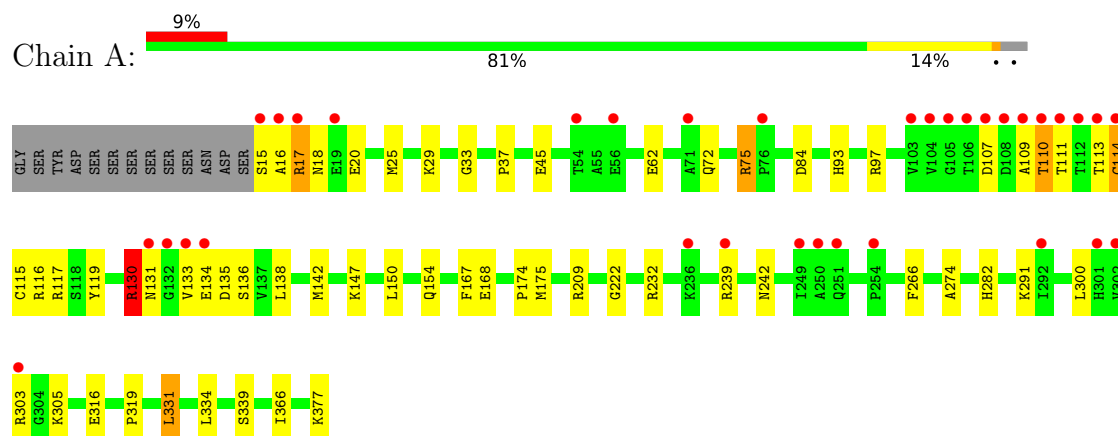
### 3 Residue-property plots [i](#)

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: stilbene O-methyltransferase



- Molecule 1: stilbene O-methyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.70Å 96.70Å 166.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.71 – 2.10 19.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.71-2.10) 99.8 (19.70-2.10)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, $R_{free}$	0.171 , 0.203 0.182 , 0.211	Depositor DCC
$R_{free}$ test set	2652 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, ACT, 1PE, GOL, NAD, 8KZ

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	0.72	1/2902 (0.0%)	0.96	3/3933 (0.1%)
1	B	0.72	2/2888 (0.1%)	1.03	9/3915 (0.2%)
All	All	0.72	3/5790 (0.1%)	0.99	12/7848 (0.2%)

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	A	0	7
1	B	0	3
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	GLU	CD-OE1	-6.07	1.19	1.25
1	B	142	MET	CG-SD	5.32	1.95	1.81
1	A	142	MET	CG-SD	5.30	1.95	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	B	142	MET	CG-SD-CE	8.79	114.26	100.20
1	B	343	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	16	ALA	CB-CA-C	6.83	120.35	110.10
1	B	57	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	114	CYS	CB-CA-C	-5.72	98.95	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	B	209	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	B	377	LYS	CA-C-O	-5.33	108.91	120.10
1	A	135	ASP	CB-CA-C	5.17	120.73	110.40
1	A	130	ARG	CB-CG-CD	5.08	124.80	111.60
1	B	359	ARG	CG-CD-NE	5.04	122.38	111.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	CYS	Peptide
1	A	130	ARG	Sidechain
1	A	209	ARG	Sidechain
1	A	232	ARG	Sidechain
1	A	239	ARG	Sidechain
1	A	303	ARG	Sidechain
1	A	75	ARG	Sidechain
1	B	130	ARG	Sidechain
1	B	17	ARG	Sidechain
1	B	317	PRO	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	2844	0	2822	50	0
1	B	2830	0	2816	54	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	10	0
4	A	36	0	48	3	0
4	B	48	0	64	10	0
5	A	8	0	12	0	0
5	B	20	0	29	10	0
6	A	4	0	3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	3	0	0
7	A	7	0	10	2	0
7	B	7	0	10	0	0
8	A	16	0	21	6	0
9	A	141	0	0	3	0
9	B	127	0	0	6	0
All	All	6216	0	5890	100	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 8.

All (100) 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:75:ARG:HG2	1:A:75:ARG:HH11	1.40	0.83
1:B:221:GLY:HA2	3:B:402:NAD:H2A	1.63	0.81
1:A:17:ARG:NH1	9:A:501:HOH:O	1.96	0.79
1:B:285:ASP:OD2	3:B:402:NAD:H4N	1.86	0.74
5:B:416:EDO:H22	9:B:574:HOH:O	1.88	0.73
5:B:404:EDO:H22	1:A:17:ARG:HB3	1.70	0.72
1:A:16:ALA:HB2	1:A:25:MET:CE	2.19	0.72
1:A:339:SER:HB3	7:A:407:PEG:H42	1.75	0.68
1:A:29:LYS:HG3	8:A:402:1PE:H162	1.76	0.68
1:B:221:GLY:CA	3:B:402:NAD:H2A	2.24	0.68
1:A:45[A]:GLU:OE2	9:A:502:HOH:O	2.14	0.66
1:B:111:THR:HG22	1:B:117:ARG:NH1	2.09	0.66
1:B:97:ARG:HG3	1:B:97:ARG:HH11	1.61	0.65
1:B:104:VAL:O	1:B:104:VAL:HG13	1.96	0.65
1:B:97:ARG:HH11	1:B:97:ARG:CG	2.11	0.64
1:B:130:ARG:O	1:B:131:ASN:HB3	1.97	0.62
5:B:417:EDO:C2	1:A:18:ASN:HD21	2.13	0.62
1:B:170:THR:HG23	4:B:407:GOL:H12	1.82	0.61
5:B:417:EDO:H21	1:A:18:ASN:HD21	1.66	0.60
1:B:130:ARG:HG2	1:B:138:LEU:CD2	2.32	0.60
1:A:84:ASP:OD2	1:A:111:THR:HG22	2.01	0.59
1:B:33:GLY:HA2	5:B:416:EDO:H21	1.84	0.59
4:A:408:GOL:H11	9:A:533:HOH:O	2.02	0.59
1:A:130:ARG:HG2	1:A:138:LEU:CD2	2.33	0.58
1:B:150:LEU:HD12	1:A:154:GLN:HE22	1.68	0.58
1:B:150:LEU:HD12	1:A:154:GLN:NE2	2.20	0.56
5:B:406:EDO:H12	1:A:29:LYS:HE3	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:417:EDO:H11	1:A:20:GLU:HG2	1.89	0.55
1:B:154:GLN:NE2	1:A:150:LEU:HD12	2.22	0.54
1:A:16:ALA:HB2	1:A:25:MET:HE3	1.89	0.54
1:B:112:THR:O	1:B:115:CYS:O	2.25	0.54
1:B:244:ASP:HA	3:B:402:NAD:N1A	2.23	0.54
3:B:402:NAD:O1A	3:B:402:NAD:H8A	2.07	0.54
1:A:168[B]:GLU:HG2	1:A:174:PRO:HA	1.89	0.54
1:B:111:THR:HG22	1:B:117:ARG:HH12	1.71	0.53
1:B:249:ILE:HG23	1:B:260:HIS:HB3	1.89	0.53
1:A:300:LEU:O	1:A:377:LYS:NZ	2.30	0.53
1:B:264:SER:HA	3:B:402:NAD:N7A	2.25	0.52
1:B:89:PHE:CG	1:A:331:LEU:HD22	2.45	0.51
1:A:154:GLN:HG3	4:A:401:GOL:H31	1.92	0.51
1:B:170:THR:CG2	4:B:407:GOL:H12	2.41	0.51
1:B:200:ILE:O	1:B:204:LEU:HB2	2.11	0.51
1:A:107:ASP:CG	1:A:116:ARG:HH22	2.14	0.51
1:B:33:GLY:HA3	8:A:402:1PE:H141	1.92	0.50
1:B:70:ALA:HB3	9:B:502:HOH:O	2.11	0.50
1:B:186:ASN:HD21	4:B:411:GOL:H32	1.76	0.50
1:B:291:LYS:HZ1	3:B:402:NAD:H6N	1.76	0.49
1:B:284:TRP:CZ3	4:B:405:GOL:H12	2.48	0.49
4:B:405:GOL:H11	9:B:565:HOH:O	2.13	0.48
5:B:417:EDO:H21	1:A:18:ASN:ND2	2.28	0.48
5:B:417:EDO:C2	1:A:18:ASN:ND2	2.77	0.48
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.17	0.48
1:A:16:ALA:HB2	1:A:25:MET:HE1	1.94	0.48
1:B:215:ASP:HB2	1:B:273:ASN:OD1	2.14	0.47
1:B:70:ALA:N	9:B:502:HOH:O	2.32	0.47
1:A:110:THR:HG21	1:A:115:CYS:O	2.14	0.47
1:A:334:LEU:HD23	1:A:334:LEU:C	2.35	0.47
1:B:285:ASP:H	3:B:402:NAD:H71N	1.62	0.47
1:B:168[B]:GLU:HG2	1:B:174:PRO:HA	1.97	0.47
1:B:197:SER:HA	1:B:278:LYS:HE3	1.96	0.46
1:B:155:ASN:ND2	4:B:407:GOL:H31	2.31	0.46
1:B:300:LEU:O	1:B:377:LYS:NZ	2.34	0.46
1:A:93:HIS:ND1	8:A:402:1PE:H221	2.31	0.45
1:A:266:PHE:O	1:A:291:LYS:NZ	2.47	0.45
1:B:183:GLY:N	1:B:184:PRO:CD	2.79	0.45
1:A:274:ALA:HA	1:A:305:LYS:O	2.16	0.45
1:A:167:PHE:CE1	1:A:175:MET:HA	2.52	0.45
1:A:111:THR:HG22	1:A:117:ARG:HH11	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:HD11	3:B:402:NAD:H3B	1.99	0.44
1:A:131:ASN:HD22	1:A:134:GLU:HG3	1.83	0.44
1:A:37:PRO:HD3	8:A:402:1PE:H141	1.98	0.44
1:B:33:GLY:HA3	8:A:402:1PE:C14	2.48	0.44
1:B:247:HIS:CD2	4:B:411:GOL:H12	2.53	0.44
1:B:22:GLU:HB2	9:B:560:HOH:O	2.17	0.43
1:B:167:PHE:CE1	1:B:175:MET:HA	2.54	0.43
1:B:16:ALA:HB1	1:A:366:ILE:O	2.19	0.43
1:A:62:GLU:HB2	1:A:109:ALA:HB1	2.00	0.43
1:A:130:ARG:HA	1:A:138:LEU:HD23	2.00	0.43
1:B:154:GLN:HE22	1:A:150:LEU:HD12	1.82	0.42
1:A:33:GLY:HA2	8:A:402:1PE:H251	2.01	0.42
1:A:16:ALA:CB	1:A:25:MET:CE	2.96	0.42
1:A:339:SER:HB3	7:A:407:PEG:C4	2.48	0.42
1:B:130:ARG:O	1:B:131:ASN:CB	2.62	0.42
1:A:131:ASN:ND2	1:A:134:GLU:HG3	2.35	0.42
1:B:112:THR:HG21	9:B:544:HOH:O	2.19	0.41
1:B:186:ASN:OD1	4:B:411:GOL:H32	2.20	0.41
1:B:216:VAL:HA	1:B:239:ARG:O	2.20	0.41
1:B:89:PHE:CD2	1:A:331:LEU:HD22	2.54	0.41
1:B:97:ARG:CG	1:B:97:ARG:NH1	2.77	0.41
1:B:114:CYS:SG	1:B:115:CYS:N	2.93	0.41
1:A:222:GLY:HA3	1:A:242:ASN:OD1	2.20	0.41
1:B:92:SER:O	1:A:319:PRO:HA	2.21	0.41
1:B:97:ARG:O	1:B:119:TYR:HA	2.21	0.41
1:A:107:ASP:CG	1:A:116:ARG:NH2	2.74	0.41
1:B:186:ASN:ND2	4:B:411:GOL:H32	2.36	0.41
1:B:151:ASP:HA	4:A:401:GOL:H11	2.03	0.40
4:B:407:GOL:O3	1:A:147:LYS:HD2	2.21	0.40
1:A:97:ARG:O	1:A:119:TYR:HA	2.21	0.40
5:B:417:EDO:H22	1:A:18:ASN:ND2	2.37	0.40
1:B:288:ALA:HB2	3:B:402:NAD:C2N	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/376 (97%)	355 (97%)	9 (2%)	1 (0%)	41	41
1	B	363/376 (96%)	354 (98%)	7 (2%)	2 (1%)	25	21
All	All	728/752 (97%)	709 (97%)	16 (2%)	3 (0%)	34	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	THR
1	B	104	VAL
1	B	131	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/312 (97%)	295 (97%)	9 (3%)	41	44
1	B	302/312 (97%)	297 (98%)	5 (2%)	60	67
All	All	606/624 (97%)	592 (98%)	14 (2%)	50	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	GLU
1	B	107	ASP
1	B	126	LYS
1	B	136	SER
1	B	282	HIS
1	A	15	SER
1	A	17	ARG
1	A	72	GLN
1	A	110	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	133	VAL
1	A	136	SER
1	A	282	HIS
1	A	316	GLU
1	A	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	251	GLN
1	A	131	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](#)

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](#)

30 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	$\# Z  > 2$
4	GOL	A	409	-	5,5,5	0.31	0	5,5,5	0.51	0
4	GOL	B	411	-	5,5,5	0.21	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ACT	A	412	-	3,3,3	2.27	1 (33%)	3,3,3	0.70	0
4	GOL	B	415	-	5,5,5	0.29	0	5,5,5	0.68	0
5	EDO	B	417	-	3,3,3	1.63	1 (33%)	2,2,2	1.99	1 (50%)
4	GOL	A	401	-	5,5,5	0.09	0	5,5,5	0.31	0
5	EDO	B	404	-	3,3,3	0.21	0	2,2,2	0.48	0
5	EDO	A	405	-	3,3,3	0.34	0	2,2,2	0.44	0
6	ACT	B	409	-	3,3,3	0.61	0	3,3,3	1.28	0
4	GOL	B	414	-	5,5,5	0.20	0	5,5,5	0.44	0
4	GOL	B	410	-	5,5,5	0.25	0	5,5,5	0.31	0
3	NAD	A	404	-	42,48,48	1.07	2 (4%)	50,73,73	1.03	4 (8%)
2	8KZ	A	403	-	19,19,19	0.42	0	25,25,25	0.62	0
5	EDO	A	411	-	3,3,3	0.45	0	2,2,2	0.88	0
7	PEG	A	407	-	6,6,6	0.91	0	5,5,5	0.44	0
5	EDO	B	408	-	3,3,3	0.20	0	2,2,2	0.48	0
4	GOL	B	405	-	5,5,5	0.39	0	5,5,5	0.68	0
4	GOL	B	407	-	5,5,5	0.18	0	5,5,5	0.93	0
7	PEG	B	413	-	6,6,6	0.72	0	5,5,5	0.46	0
4	GOL	A	406	-	5,5,5	0.20	0	5,5,5	0.17	0
8	1PE	A	402	-	15,15,15	0.43	0	14,14,14	0.42	0
5	EDO	B	416	-	3,3,3	0.25	0	2,2,2	0.80	0
4	GOL	B	403	-	5,5,5	0.10	0	5,5,5	0.39	0
4	GOL	A	413	-	5,5,5	0.10	0	5,5,5	0.43	0
5	EDO	B	406	-	3,3,3	0.08	0	2,2,2	0.22	0
4	GOL	B	412	-	5,5,5	0.16	0	5,5,5	0.54	0
3	NAD	B	402	-	42,48,48	1.02	1 (2%)	50,73,73	1.33	6 (12%)
4	GOL	A	410	-	5,5,5	0.21	0	5,5,5	0.50	0
2	8KZ	B	401	-	19,19,19	0.65	0	25,25,25	0.66	0
4	GOL	A	408	-	5,5,5	0.33	0	5,5,5	0.42	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
4	GOL	A	409	-	-	2/4/4/4	-
4	GOL	B	411	-	-	2/4/4/4	-
4	GOL	B	415	-	-	4/4/4/4	-
5	EDO	B	417	-	-	1/1/1/1	-
4	GOL	A	401	-	-	4/4/4/4	-
5	EDO	B	404	-	-	1/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	405	-	-	1/1/1/1	-
4	GOL	B	414	-	-	3/4/4/4	-
4	GOL	B	410	-	-	0/4/4/4	-
3	NAD	A	404	-	-	1/26/62/62	0/5/5/5
2	8KZ	A	403	-	-	0/7/7/7	0/2/2/2
5	EDO	A	411	-	-	1/1/1/1	-
7	PEG	A	407	-	-	2/4/4/4	-
5	EDO	B	408	-	-	1/1/1/1	-
4	GOL	B	405	-	-	2/4/4/4	-
4	GOL	B	407	-	-	2/4/4/4	-
7	PEG	B	413	-	-	1/4/4/4	-
4	GOL	A	406	-	-	2/4/4/4	-
8	1PE	A	402	-	-	9/13/13/13	-
5	EDO	B	416	-	-	1/1/1/1	-
4	GOL	B	403	-	-	2/4/4/4	-
4	GOL	A	413	-	-	2/4/4/4	-
5	EDO	B	406	-	-	1/1/1/1	-
4	GOL	B	412	-	-	3/4/4/4	-
3	NAD	B	402	-	-	15/26/62/62	0/5/5/5
4	GOL	A	410	-	-	4/4/4/4	-
2	8KZ	B	401	-	-	0/7/7/7	0/2/2/2
4	GOL	A	408	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAD	C2N-N1N	4.57	1.40	1.35
3	A	404	NAD	O4D-C1D	4.22	1.47	1.41
6	A	412	ACT	OXT-C	-3.60	1.13	1.30
3	A	404	NAD	C2N-N1N	3.42	1.39	1.35
5	B	417	EDO	O1-C1	-2.54	1.29	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAD	PN-O3-PA	4.74	149.10	132.83
3	A	404	NAD	C6N-N1N-C2N	-3.22	119.04	121.97
3	B	402	NAD	C6N-N1N-C2N	-3.03	119.22	121.97
3	B	402	NAD	C3N-C7N-N7N	2.57	120.83	117.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	417	EDO	O1-C1-C2	-2.54	93.60	111.91
3	B	402	NAD	C5A-C6A-N6A	2.51	124.16	120.35
3	B	402	NAD	O2D-C2D-C1D	-2.47	101.75	110.85
3	A	404	NAD	C5A-C6A-N6A	2.39	123.99	120.35
3	A	404	NAD	C2N-C3N-C4N	2.38	120.95	118.26
3	A	404	NAD	O2N-PN-O1N	2.20	123.12	112.24
3	B	402	NAD	O2D-C2D-C3D	2.08	118.55	111.82

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	NAD	C5B-O5B-PA-O1A
3	B	402	NAD	C5D-O5D-PN-O1N
3	B	402	NAD	C2N-C3N-C7N-O7N
3	B	402	NAD	C2N-C3N-C7N-N7N
4	B	403	GOL	C1-C2-C3-O3
4	B	407	GOL	O1-C1-C2-C3
4	B	411	GOL	O1-C1-C2-C3
4	B	412	GOL	C1-C2-C3-O3
4	B	412	GOL	O2-C2-C3-O3
4	B	415	GOL	O1-C1-C2-O2
4	B	415	GOL	O1-C1-C2-C3
4	B	415	GOL	C1-C2-C3-O3
4	A	401	GOL	O1-C1-C2-O2
4	A	401	GOL	O1-C1-C2-C3
4	A	401	GOL	C1-C2-C3-O3
4	A	406	GOL	C1-C2-C3-O3
4	A	409	GOL	C1-C2-C3-O3
4	A	410	GOL	O1-C1-C2-C3
3	B	402	NAD	C4N-C3N-C7N-N7N
3	B	402	NAD	C4N-C3N-C7N-O7N
4	B	411	GOL	O1-C1-C2-O2
4	A	409	GOL	O2-C2-C3-O3
8	A	402	1PE	OH2-C12-C22-OH3
8	A	402	1PE	OH7-C16-C26-OH6
4	B	405	GOL	C1-C2-C3-O3
4	B	414	GOL	C1-C2-C3-O3
4	A	408	GOL	O1-C1-C2-C3
4	A	410	GOL	C1-C2-C3-O3
4	A	413	GOL	C1-C2-C3-O3
4	B	403	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

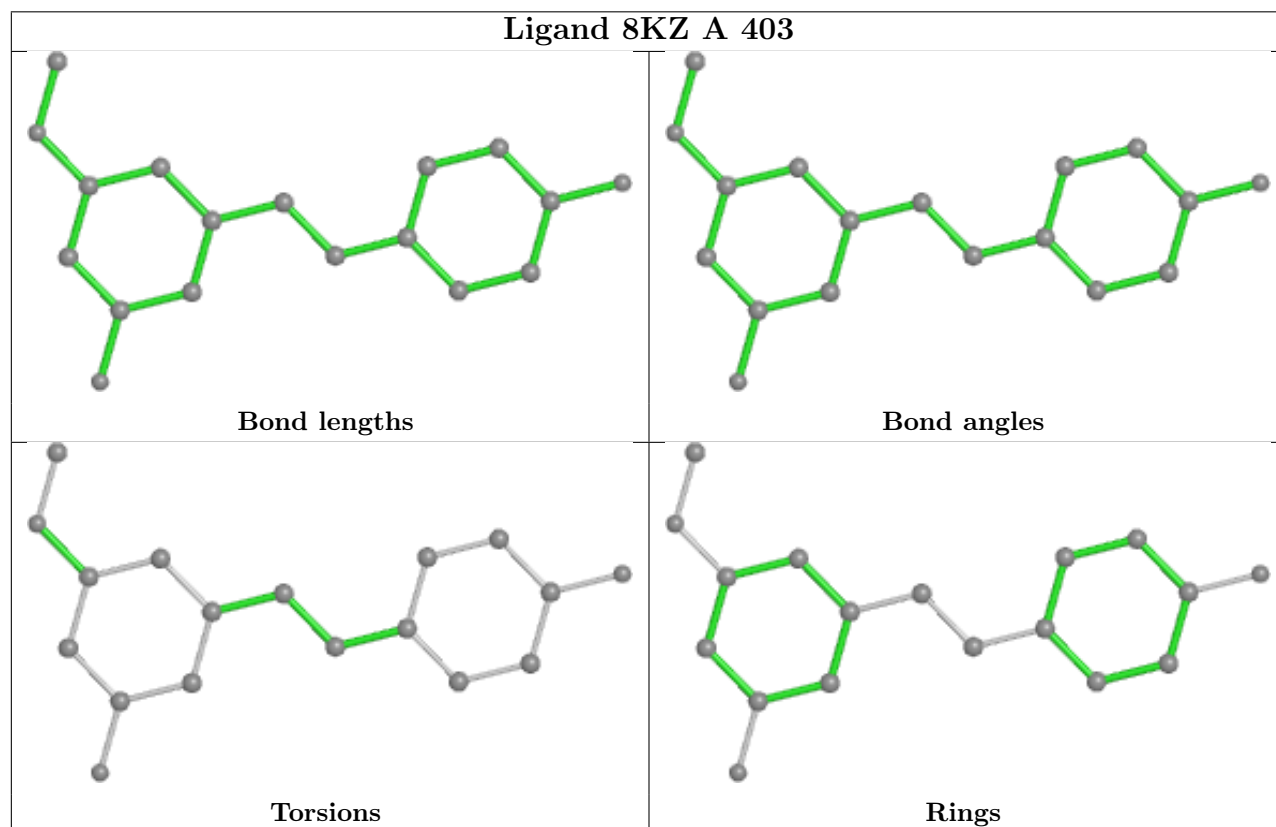
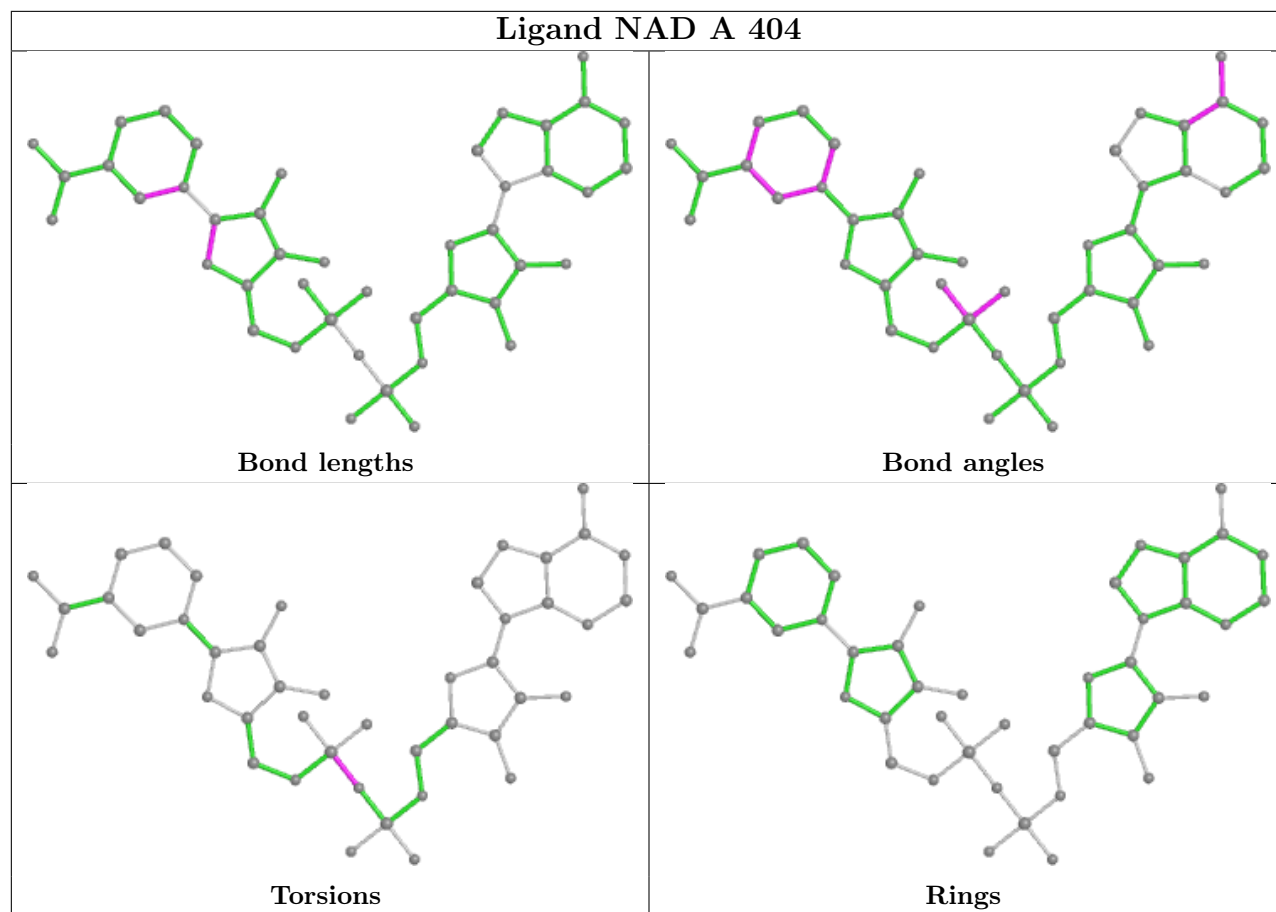
Mol	Chain	Res	Type	Atoms
4	B	407	GOL	O1-C1-C2-O2
4	B	414	GOL	O2-C2-C3-O3
4	B	415	GOL	O2-C2-C3-O3
4	A	406	GOL	O2-C2-C3-O3
3	B	402	NAD	C3B-C4B-C5B-O5B
3	B	402	NAD	C3D-C4D-C5D-O5D
5	B	408	EDO	O1-C1-C2-O2
5	B	416	EDO	O1-C1-C2-O2
5	B	417	EDO	O1-C1-C2-O2
8	A	402	1PE	OH6-C15-C25-OH5
8	A	402	1PE	OH4-C13-C23-OH3
4	B	405	GOL	O2-C2-C3-O3
4	A	401	GOL	O2-C2-C3-O3
4	A	410	GOL	O1-C1-C2-O2
7	B	413	PEG	O2-C3-C4-O4
4	B	414	GOL	O1-C1-C2-O2
4	A	408	GOL	O1-C1-C2-O2
4	A	410	GOL	O2-C2-C3-O3
3	B	402	NAD	O4D-C4D-C5D-O5D
3	B	402	NAD	PN-O3-PA-O5B
8	A	402	1PE	C13-C23-OH3-C22
3	B	402	NAD	C4B-C5B-O5B-PA
4	B	412	GOL	O1-C1-C2-O2
8	A	402	1PE	C24-C14-OH5-C25
8	A	402	1PE	C14-C24-OH4-C13
5	B	406	EDO	O1-C1-C2-O2
3	B	402	NAD	O4B-C4B-C5B-O5B
5	B	404	EDO	O1-C1-C2-O2
5	A	411	EDO	O1-C1-C2-O2
3	B	402	NAD	PN-O3-PA-O1A
8	A	402	1PE	C15-C25-OH5-C14
8	A	402	1PE	C12-C22-OH3-C23
7	A	407	PEG	C1-C2-O2-C3
5	A	405	EDO	O1-C1-C2-O2
7	A	407	PEG	O2-C3-C4-O4
4	A	413	GOL	O2-C2-C3-O3
3	B	402	NAD	C4D-C5D-O5D-PN
3	B	402	NAD	C5B-O5B-PA-O3
3	A	404	NAD	PA-O3-PN-O2N

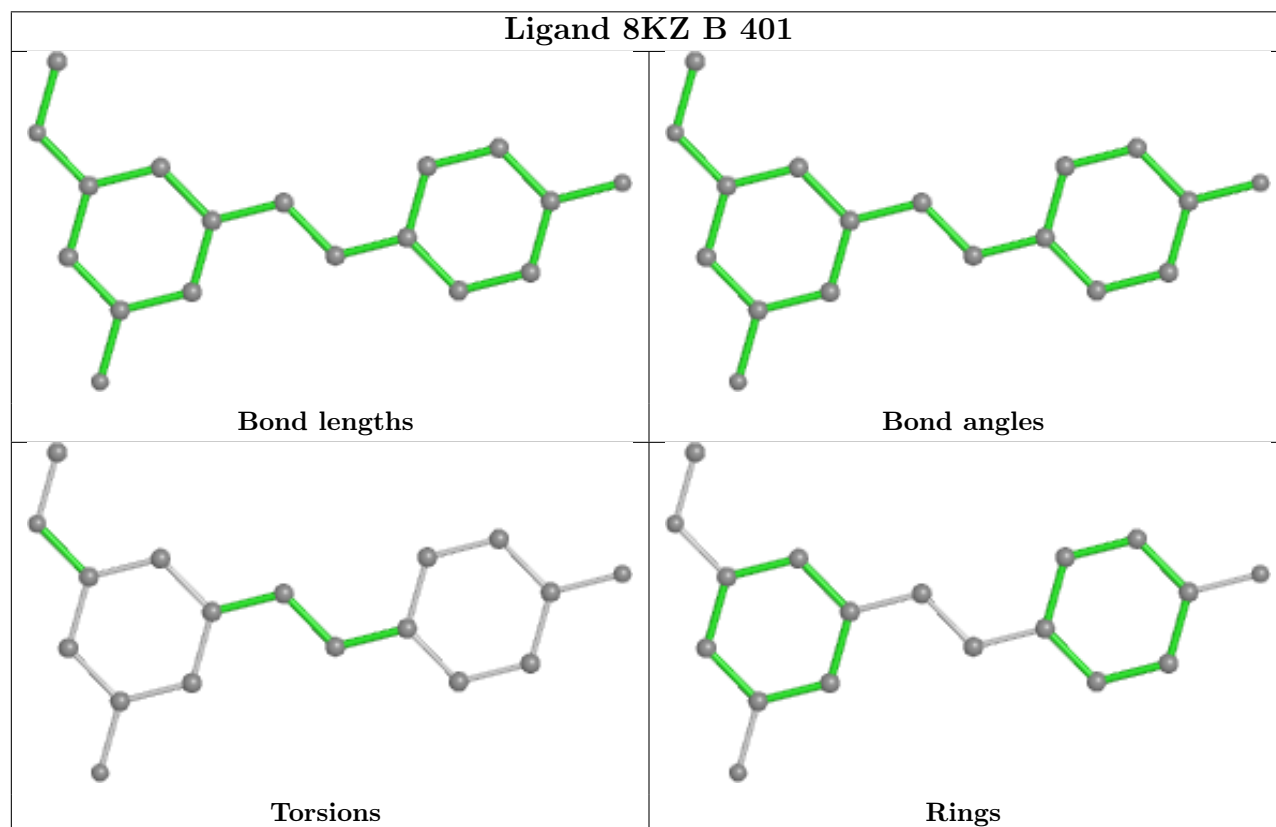
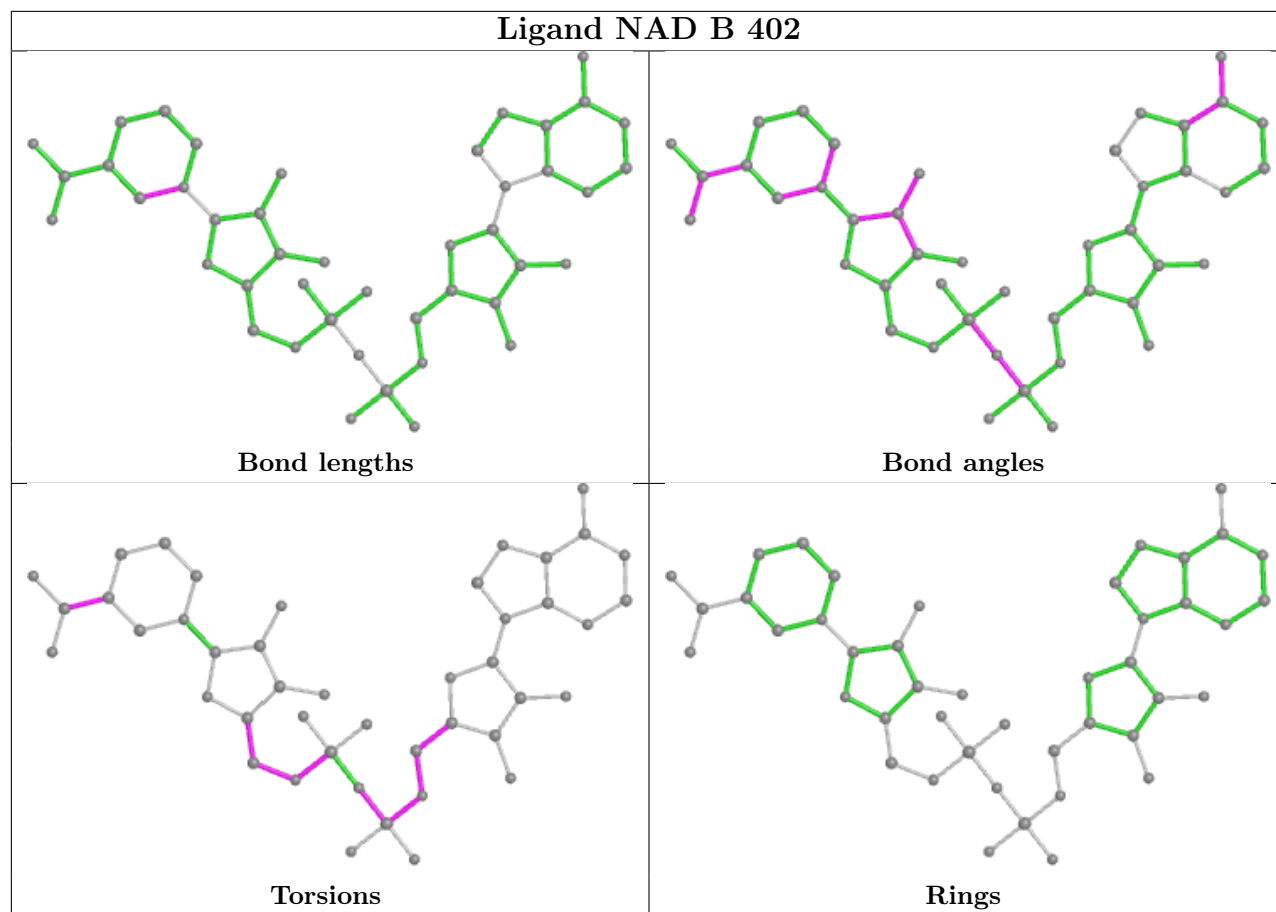
There are no ring outliers.

12 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	411	GOL	4	0
5	B	417	EDO	6	0
4	A	401	GOL	2	0
5	B	404	EDO	1	0
7	A	407	PEG	2	0
4	B	405	GOL	2	0
4	B	407	GOL	4	0
8	A	402	1PE	6	0
5	B	416	EDO	2	0
5	B	406	EDO	1	0
3	B	402	NAD	10	0
4	A	408	GOL	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	363/376 (96%)	0.22	34 (9%) <b>8</b> <b>11</b>	21, 32, 71, 128	0
1	B	362/376 (96%)	0.07	25 (6%) <b>16</b> <b>21</b>	22, 30, 65, 140	0
All	All	725/752 (96%)	0.14	59 (8%) <b>12</b> <b>15</b>	21, 31, 70, 140	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	THR	14.1
1	B	133	VAL	14.0
1	B	107	ASP	13.9
1	A	133	VAL	12.7
1	A	107	ASP	12.7
1	A	109	ALA	9.4
1	A	105	GLY	8.7
1	B	108	ASP	8.3
1	B	106	THR	8.1
1	B	109	ALA	7.6
1	B	105	GLY	7.5
1	A	108	ASP	7.1
1	B	110	THR	6.1
1	A	113	THR	5.7
1	B	104	VAL	5.5
1	A	16	ALA	5.4
1	A	15	SER	5.2
1	A	302	VAL	5.1
1	A	250	ALA	5.0
1	B	132	GLY	4.9
1	A	132	GLY	4.8
1	A	104	VAL	4.6
1	A	131	ASN	4.6
1	B	131	ASN	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	113	THR	4.1
1	B	112	THR	4.0
1	A	112	THR	3.8
1	B	16	ALA	3.8
1	A	56	GLU	3.7
1	B	56	GLU	3.5
1	A	301	HIS	3.5
1	A	110	THR	3.5
1	A	134	GLU	3.4
1	A	251	GLN	3.4
1	B	134	GLU	3.4
1	B	111	THR	3.3
1	B	19	GLU	3.3
1	B	72	GLN	3.3
1	B	114	CYS	3.3
1	A	114	CYS	3.1
1	A	236	LYS	3.0
1	B	303	ARG	3.0
1	A	254	PRO	3.0
1	A	249	ILE	2.9
1	A	111	THR	2.7
1	A	103	VAL	2.6
1	B	213	GLY	2.6
1	A	71	ALA	2.5
1	A	54	THR	2.5
1	B	281	LEU	2.4
1	A	19	GLU	2.3
1	B	256	GLU	2.2
1	A	292	ILE	2.2
1	B	70	ALA	2.1
1	A	76	PRO	2.1
1	A	17	ARG	2.1
1	A	239	ARG	2.1
1	B	103	VAL	2.0
1	A	303	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

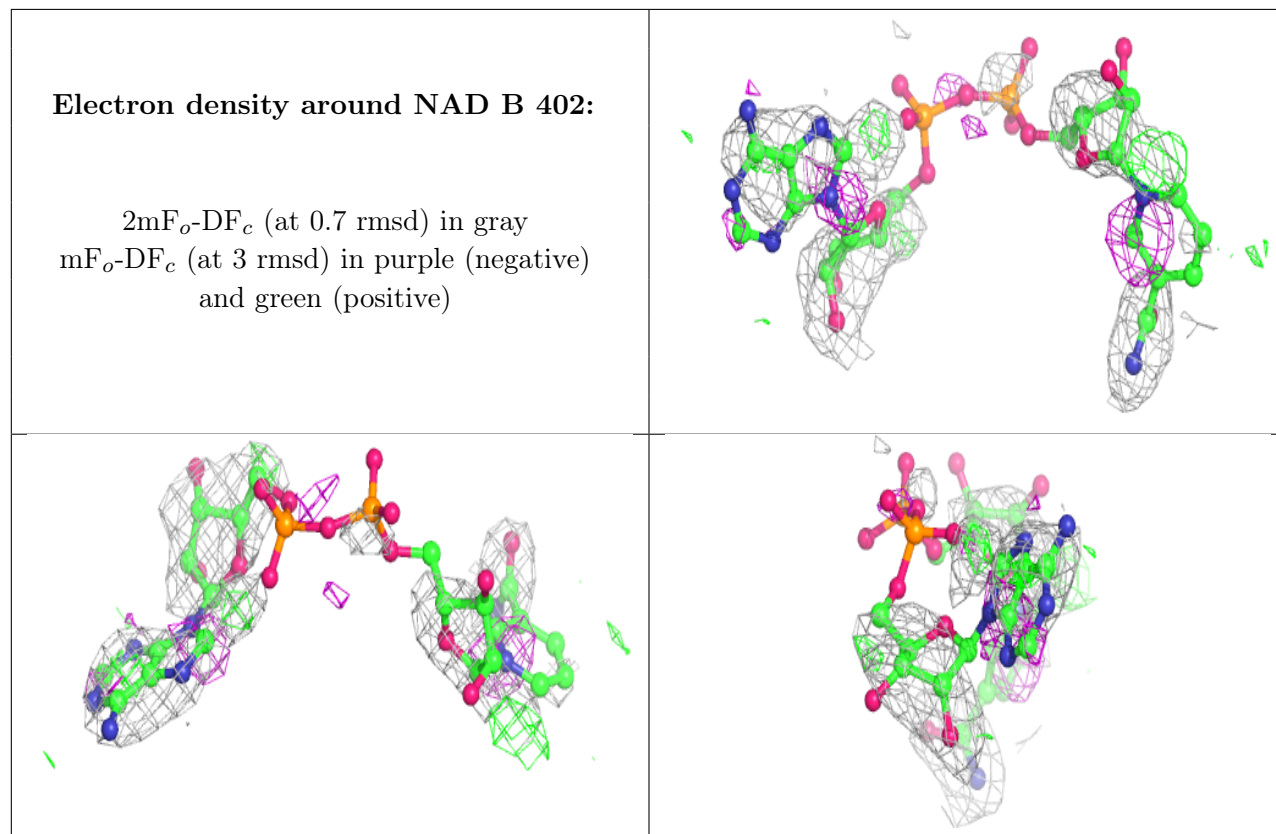
## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GOL	A	410	6/6	0.61	0.29	64,79,83,84	0
4	GOL	B	411	6/6	0.64	0.30	59,72,89,102	0
3	NAD	B	402	44/44	0.67	0.47	31,102,156,163	0
7	PEG	B	413	7/7	0.71	0.20	53,66,71,74	0
7	PEG	A	407	7/7	0.76	0.21	46,54,70,71	0
5	EDO	B	406	4/4	0.78	0.38	66,77,90,93	0
4	GOL	B	403	6/6	0.79	0.20	44,60,64,73	0
5	EDO	A	411	4/4	0.79	0.27	72,72,73,75	0
4	GOL	B	415	6/6	0.80	0.21	67,73,80,97	0
4	GOL	B	414	6/6	0.81	0.20	46,73,73,78	0
4	GOL	B	405	6/6	0.84	0.26	51,52,65,67	0
4	GOL	A	401	6/6	0.85	0.34	59,68,77,82	0
4	GOL	B	407	6/6	0.85	0.33	60,66,68,74	0
3	NAD	A	404	44/44	0.86	0.20	31,52,62,68	0
4	GOL	A	409	6/6	0.87	0.20	38,50,56,73	0
5	EDO	A	405	4/4	0.89	0.24	40,49,61,67	0
5	EDO	B	408	4/4	0.89	0.15	54,61,64,70	0
8	1PE	A	402	16/16	0.89	0.15	35,63,84,94	0
4	GOL	A	406	6/6	0.93	0.19	37,48,57,62	0
4	GOL	B	410	6/6	0.93	0.12	36,39,44,44	0
2	8KZ	B	401	18/18	0.94	0.09	22,27,31,34	0
4	GOL	B	412	6/6	0.94	0.10	41,48,58,59	0
4	GOL	A	408	6/6	0.94	0.15	37,40,44,59	0
4	GOL	A	413	6/6	0.95	0.11	32,49,58,67	0
5	EDO	B	416	4/4	0.96	0.11	39,41,43,44	0
6	ACT	B	409	4/4	0.96	0.15	32,39,44,48	0
6	ACT	A	412	4/4	0.96	0.14	30,34,35,39	0
5	EDO	B	417	4/4	0.97	0.28	33,41,52,56	0
2	8KZ	A	403	18/18	0.97	0.11	21,25,30,33	0
5	EDO	B	404	4/4	0.98	0.11	43,50,56,58	0

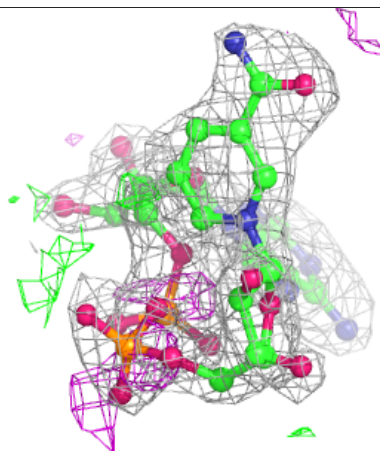
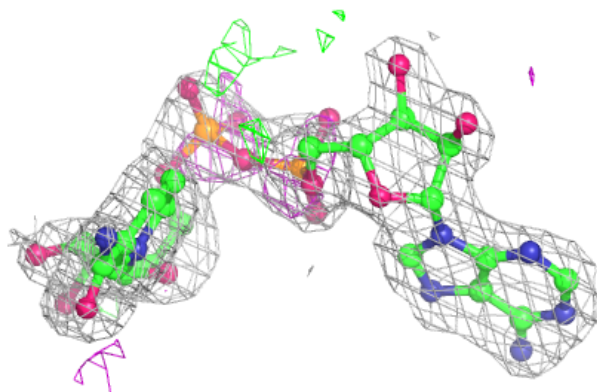
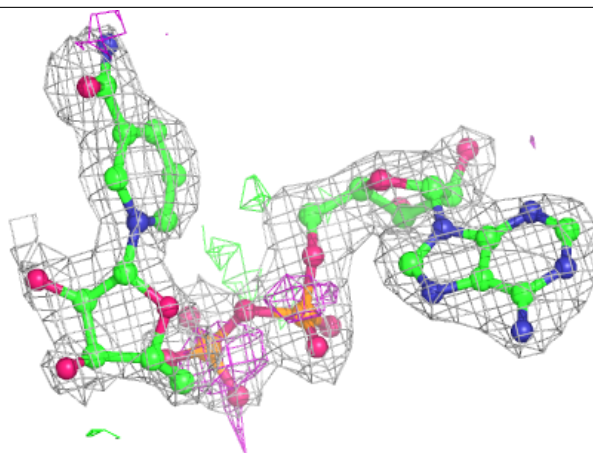
The following is a graphical depiction of the model fit to experimental electron density of all

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.

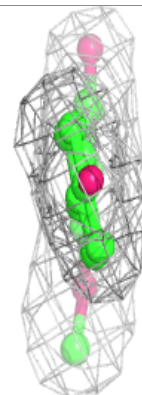
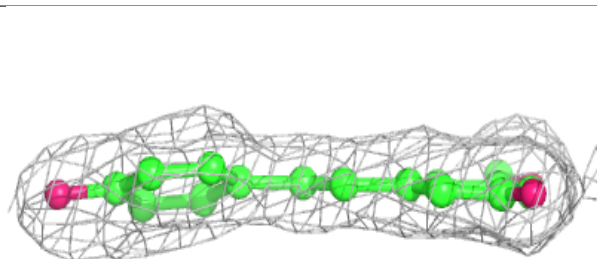
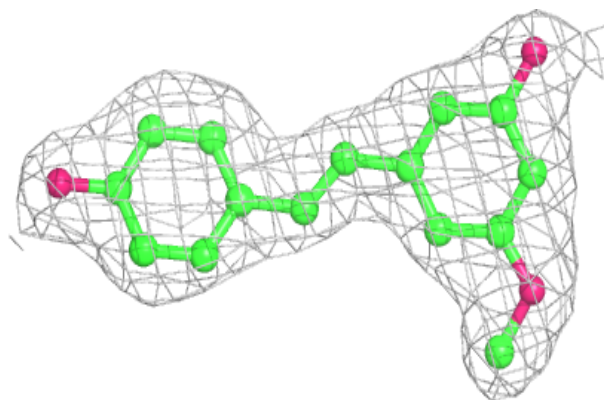


**Electron density around NAD A 404:**

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

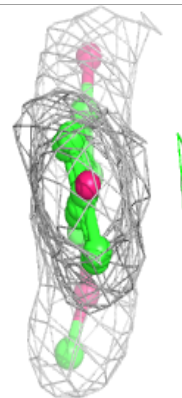
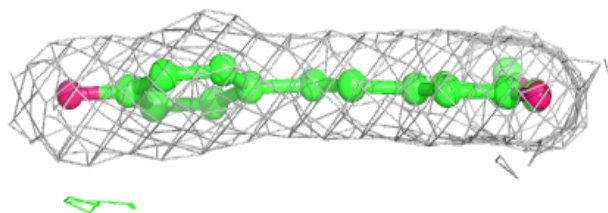
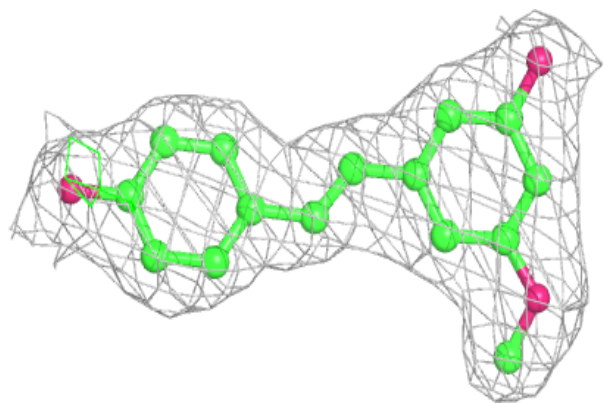
**Electron density around 8KZ B 401:**

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



**Electron density around 8KZ A 403:**

$2mF_o - DF_c$  (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.