



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2023 – 02:18 PM JST

PDB ID : 5H4D  
Title : Crystal structure of hSIRT3 in complex with a specific agonist Amiodarone hydrochloride  
Authors : Zhang, S.; Fu, L.; Liu, J.; Liu, B.  
Deposited on : 2016-10-31  
Resolution : 3.21 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 : 2.32.2  
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) : 2.32.2

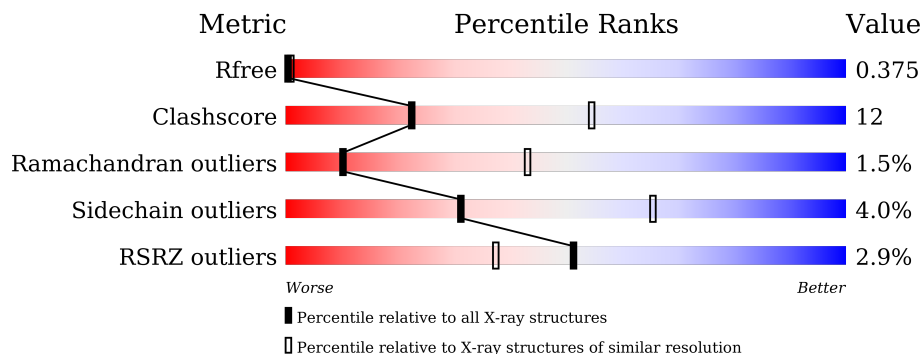
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	271	
1	H	271	
2	C	4	
2	D	4	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	401	-	-	X	-
5	BBI	A	403	-	-	-	X
5	BBI	H	405	-	-	-	X
6	NAD	A	404	-	-	-	X
8	PEG	H	401	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4526 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	Total 2127	C 1370	N 366	O 382	S 9	0	0	0
1	H	271	Total 2121	C 1364	N 366	O 382	S 9	0	0	0

- Molecule 2 is a protein called ARG-HIS-LYS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	4	Total 42	C 26	N 11	O 5	0	0	0
2	C	4	Total 42	C 26	N 11	O 5	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0

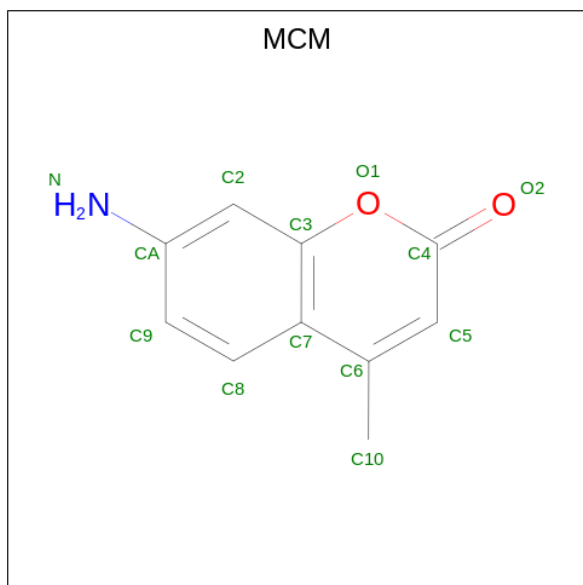
- Molecule 5 is (2-butyl-1-benzofuran-3-yl){4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl}methanone (three-letter code: BBI) (formula: C<sub>25</sub>H<sub>29</sub>I<sub>2</sub>NO<sub>3</sub>).



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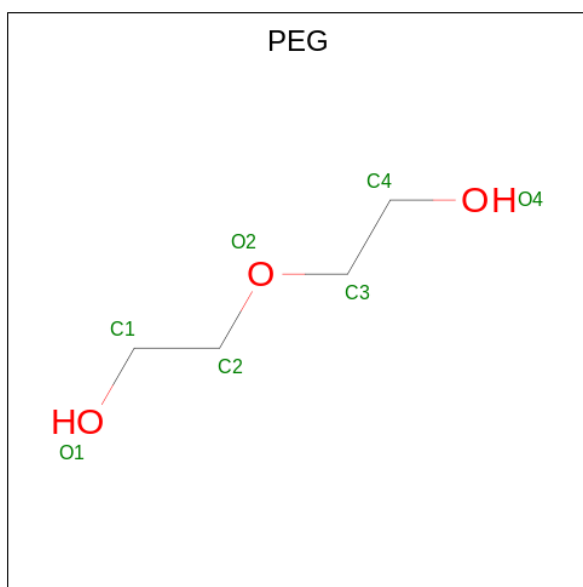
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
6	H	1	44	21	7	14	2	0	0

- Molecule 7 is 7-AMINO-4-METHYL-CHROMEN-2-ONE (three-letter code: MCM) (formula: C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	D	1	13	10	1	2	0	0
7	C	1	13	10	1	2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).

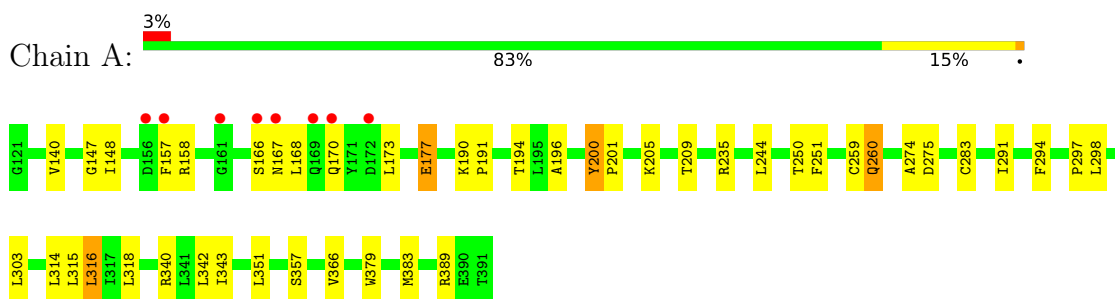


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 7 4 3	0	0
8	H	1	Total C O 7 4 3	0	0

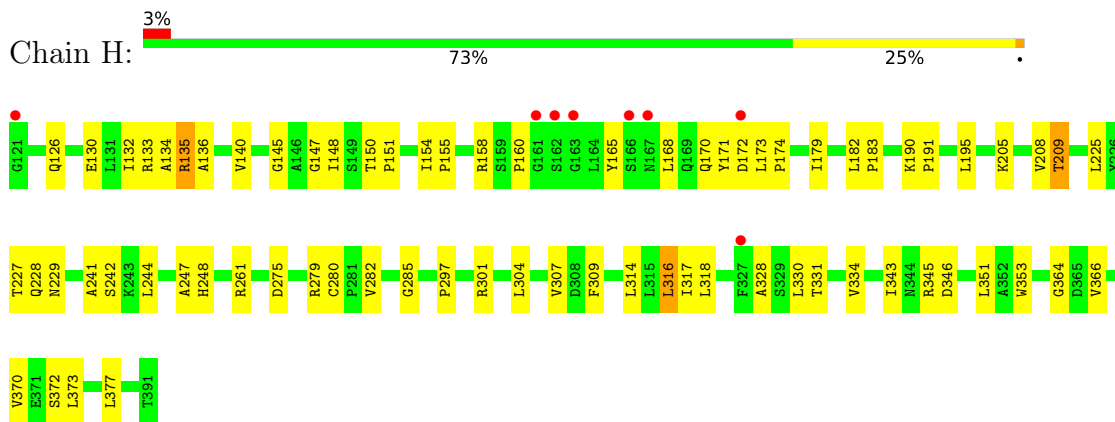
### 3 Residue-property plots

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: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



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- Molecule 2: ARG-HIS-LYS



- Molecule 2: ARG-HIS-LYS





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.56Å 114.56Å 123.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.32 – 3.21 38.66 – 3.21	Depositor EDS
% Data completeness (in resolution range)	59.2 (77.32-3.21) 59.2 (38.66-3.21)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.213 , 0.372 0.221 , 0.375	Depositor DCC
$R_{free}$ test set	285 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtrriage
Anisotropy	0.336	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 10.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.349 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	4526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% 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: PEG, NAD, ALY, BBI, MG, MCM, ZN

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	0.38	0/2182	0.58	0/2974
1	H	0.39	0/2175	0.63	0/2965
2	C	0.52	0/30	0.70	0/37
2	D	0.46	0/30	0.68	0/37
All	All	0.39	0/4417	0.61	0/6013

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
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	LYS	Mainchain

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2127	0	2137	30	0
1	H	2121	0	2130	54	0
2	C	42	0	49	4	0
2	D	42	0	48	6	1
3	A	1	0	0	2	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	H	1	0	0	0	0
5	A	31	0	29	6	1
5	H	31	0	29	14	0
6	A	44	0	26	2	0
6	H	44	0	26	10	0
7	C	13	0	8	3	0
7	D	13	0	8	3	0
8	H	14	0	20	8	0
All	All	4526	0	4510	105	1

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 12.

All (105) 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:H:405:BBI:H25	5:H:405:BBI:H30	1.42	1.00
2:D:4:ALY:OH	5:H:405:BBI:H23	1.69	0.93
1:A:259:CYS:HG	3:A:401:ZN:ZN	0.71	0.90
1:H:228:GLN:O	6:H:406:NAD:O2D	1.95	0.85
1:H:241:ALA:O	8:H:401:PEG:H21	1.80	0.80
1:H:228:GLN:O	6:H:406:NAD:C2D	2.31	0.78
5:H:405:BBI:IBD	5:H:405:BBI:H18	2.58	0.74
5:H:405:BBI:H24	6:H:406:NAD:H4D	1.71	0.72
1:H:366:VAL:HG23	6:H:406:NAD:C2A	2.22	0.70
1:H:158:ARG:CZ	5:H:405:BBI:H28	2.23	0.69
1:H:248:HIS:CD2	6:H:406:NAD:O3D	2.46	0.69
1:A:259:CYS:SG	3:A:401:ZN:ZN	1.81	0.68
1:H:134:ALA:O	1:H:136:ALA:N	2.27	0.68
2:D:4:ALY:O	7:D:101:MCM:H9	1.97	0.63
1:H:366:VAL:HG23	6:H:406:NAD:H2A	1.81	0.62
1:A:158:ARG:HD3	5:A:403:BBI:H25	1.80	0.62
2:D:4:ALY:O	7:D:101:MCM:C9	2.45	0.61
1:H:228:GLN:O	6:H:406:NAD:H2D	2.00	0.61
5:A:403:BBI:H19	5:A:403:BBI:IAS	2.74	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:HG23	6:A:404:NAD:C2A	2.34	0.57
1:H:140:VAL:HG22	1:H:314:LEU:HD23	1.85	0.57
1:A:168:LEU:HB3	1:A:173:LEU:HD12	1.86	0.57
5:A:403:BBI:IAS	5:A:403:BBI:CAW	3.23	0.57
2:C:4:ALY:O	7:C:101:MCM:H9	2.04	0.57
1:H:317:ILE:HD13	1:H:351:LEU:HD11	1.87	0.56
1:H:209:THR:HG23	1:H:370:VAL:HG21	1.88	0.55
1:H:173:LEU:HD11	1:H:179:ILE:HG23	1.89	0.55
1:H:148:ILE:HG22	1:H:209:THR:HG21	1.89	0.54
1:A:342:LEU:HD22	1:A:351:LEU:HD12	1.89	0.54
1:H:345:ARG:HA	1:H:364:GLY:O	2.07	0.53
1:A:147:GLY:HA2	6:A:404:NAD:C8A	2.37	0.53
1:H:316:LEU:HD22	1:H:318:LEU:HG	1.90	0.52
1:H:261:ARG:CZ	1:H:282:VAL:HG11	2.40	0.52
5:H:405:BBI:H24	6:H:406:NAD:C4D	2.37	0.52
1:H:145:GLY:O	1:H:229:ASN:ND2	2.41	0.52
1:A:148:ILE:HG22	1:A:209:THR:HG21	1.92	0.51
1:H:158:ARG:NE	5:H:405:BBI:H28	2.25	0.51
5:H:405:BBI:CBE	5:H:405:BBI:H13	2.41	0.51
1:H:309:PHE:CE2	1:H:330:LEU:HB3	2.46	0.51
1:A:294:PHE:HZ	5:A:403:BBI:H22	1.75	0.51
1:A:251:PHE:CE2	1:A:291:ILE:HD11	2.47	0.50
1:H:171:TYR:O	1:H:173:LEU:N	2.44	0.50
2:D:3:LYS:O	2:D:4:ALY:C	2.59	0.49
2:C:4:ALY:O	7:C:101:MCM:C9	2.57	0.49
1:H:331:THR:O	1:H:334:VAL:HG22	2.12	0.49
1:H:229:ASN:HA	6:H:406:NAD:H2N	1.92	0.49
2:D:4:ALY:OH	5:H:405:BBI:CBB	2.52	0.48
1:H:182:LEU:HB2	1:H:183:PRO:HD3	1.95	0.48
1:A:379:TRP:O	1:A:383:MET:HB2	2.13	0.48
5:H:405:BBI:IBD	5:H:405:BBI:CAW	3.31	0.48
1:H:316:LEU:HD22	1:H:318:LEU:CD2	2.44	0.47
1:H:126:GLN:O	1:H:130:GLU:HG2	2.14	0.47
1:A:260:GLN:HE21	1:A:260:GLN:HA	1.80	0.47
1:A:235:ARG:HG3	1:A:244:LEU:CD1	2.45	0.47
1:H:150:THR:HG22	1:H:154:ILE:O	2.15	0.47
5:A:403:BBI:IAS	5:A:403:BBI:H18	2.85	0.46
1:H:147:GLY:HA2	6:H:406:NAD:C8A	2.46	0.46
1:H:261:ARG:NH2	1:H:282:VAL:HG11	2.30	0.46
1:H:301:ARG:NE	8:H:401:PEG:H22	2.31	0.46
1:A:190:LYS:O	1:A:194:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HD22	1:A:318:LEU:HG	1.98	0.46
1:A:298:LEU:HD12	2:C:2:HIS:HB3	1.97	0.45
1:A:274:ALA:O	1:A:275:ASP:HB2	2.17	0.45
2:D:3:LYS:HA	1:H:297:PRO:HA	1.99	0.45
1:H:225:LEU:HD23	1:H:244:LEU:CD2	2.47	0.45
1:H:280:CYS:N	1:H:285:GLY:O	2.46	0.45
1:H:242:SER:O	8:H:401:PEG:O1	2.35	0.44
5:H:405:BBI:H30	5:H:405:BBI:CBB	2.21	0.44
1:A:297:PRO:HA	2:C:3:LYS:HA	2.00	0.44
7:C:101:MCM:H101	7:C:101:MCM:H8	1.75	0.44
1:A:177:GLU:HG2	5:A:403:BBI:IBD	2.87	0.44
1:H:301:ARG:HE	8:H:401:PEG:C2	2.31	0.44
1:H:301:ARG:HE	8:H:401:PEG:H22	1.81	0.44
1:A:251:PHE:CD2	1:A:291:ILE:HD11	2.53	0.44
1:H:160:PRO:HA	1:H:165:TYR:CE1	2.52	0.44
5:H:405:BBI:CBB	5:H:405:BBI:CAZ	2.87	0.44
1:A:318:LEU:HD21	1:A:343:ILE:HD12	2.00	0.43
1:A:173:LEU:HD11	1:A:191:PRO:HB3	1.99	0.43
1:H:168:LEU:HD23	1:H:171:TYR:CD2	2.53	0.43
1:H:343:ILE:HD11	1:H:373:LEU:HD22	2.00	0.43
1:A:318:LEU:HD23	1:A:343:ILE:HB	2.00	0.43
1:A:303:LEU:HD21	1:H:307:VAL:HG13	2.01	0.43
1:H:301:ARG:NH2	1:H:304:LEU:HD11	2.34	0.42
1:A:140:VAL:HG22	1:A:314:LEU:HD23	2.00	0.42
1:A:196:ALA:O	1:A:200:TYR:N	2.52	0.42
1:H:132:ILE:O	1:H:135:ARG:NH2	2.52	0.42
1:H:150:THR:OG1	1:H:151:PRO:HD3	2.20	0.42
1:H:190:LYS:N	1:H:191:PRO:CD	2.83	0.42
5:H:405:BBI:CAV	5:H:405:BBI:IAS	3.38	0.42
1:H:160:PRO:HA	1:H:165:TYR:CD1	2.55	0.42
1:A:315:LEU:HB3	1:A:340:ARG:HA	2.01	0.42
1:H:241:ALA:O	8:H:401:PEG:C2	2.59	0.42
1:H:301:ARG:NE	8:H:401:PEG:C2	2.82	0.41
1:H:279:ARG:HA	1:H:285:GLY:O	2.20	0.41
1:H:133:ARG:HG3	1:H:377:LEU:HD23	2.03	0.41
5:H:405:BBI:IAS	5:H:405:BBI:H17	2.91	0.41
1:A:190:LYS:N	1:A:191:PRO:CD	2.84	0.41
1:H:316:LEU:HD13	1:H:318:LEU:HD11	2.02	0.41
1:A:140:VAL:CG2	1:A:314:LEU:HD23	2.51	0.41
7:D:101:MCM:H8	7:D:101:MCM:H101	1.71	0.41
1:H:353:TRP:HA	1:H:353:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:THR:O	1:H:247:ALA:HB3	2.21	0.41
1:H:244:LEU:C	8:H:401:PEG:H11	2.42	0.41
1:A:259:CYS:SG	1:A:283:CYS:SG	3.20	0.40
1:H:150:THR:N	1:H:151:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:ARG:NE	5:A:403:BBI:OAO[5_555]	2.15	0.05

## 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	269/271 (99%)	234 (87%)	33 (12%)	2 (1%)	22	60
1	H	269/271 (99%)	240 (89%)	23 (9%)	6 (2%)	6	34
2	C	2/4 (50%)	2 (100%)	0	0	100	100
2	D	2/4 (50%)	2 (100%)	0	0	100	100
All	All	542/550 (98%)	478 (88%)	56 (10%)	8 (2%)	10	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	135	ARG
1	H	172	ASP
1	A	157	PHE
1	H	275	ASP
1	H	328	ALA
1	H	155	PRO

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Mol	Chain	Res	Type
1	H	174	PRO
1	A	201	PRO

### 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	235/235 (100%)	224 (95%)	11 (5%)	26	61
1	H	234/235 (100%)	226 (97%)	8 (3%)	37	69
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	475/476 (100%)	456 (96%)	19 (4%)	31	65

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

Mol	Chain	Res	Type
1	A	166	SER
1	A	167	ASN
1	A	170	GLN
1	A	177	GLU
1	A	200	TYR
1	A	205	LYS
1	A	250	THR
1	A	260	GLN
1	A	316	LEU
1	A	357	SER
1	A	389	ARG
1	H	170	GLN
1	H	195	LEU
1	H	205	LYS
1	H	208	VAL
1	H	209	THR
1	H	316	LEU
1	H	346	ASP
1	H	372	SER

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

Mol	Chain	Res	Type
1	A	167	ASN
1	A	169	GLN
1	A	170	GLN
1	A	260	GLN
1	H	248	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	ALY	C	4	2,7	10,11,12	0.67	0	7,12,14	0.93	0
2	ALY	D	4	2,7	10,11,12	0.64	0	7,12,14	0.84	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	ALY	C	4	2,7	-	0/9/10/12	-
2	ALY	D	4	2,7	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	ALY	2	0
2	D	4	ALY	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
5	BBI	H	405	-	27,33,33	3.01	4 (14%)	36,45,45	1.01	1 (2%)
6	NAD	H	406	-	42,48,48	0.98	2 (4%)	50,73,73	1.37	5 (10%)
5	BBI	A	403	-	27,33,33	3.22	4 (14%)	36,45,45	1.39	7 (19%)
7	MCM	C	101	2	12,14,14	1.96	1 (8%)	16,20,20	2.25	4 (25%)
8	PEG	H	403	-	6,6,6	0.54	0	5,5,5	0.20	0
7	MCM	D	101	2	12,14,14	1.90	1 (8%)	16,20,20	1.98	4 (25%)
6	NAD	A	404	-	42,48,48	0.92	3 (7%)	50,73,73	1.20	5 (10%)
8	PEG	H	401	-	6,6,6	0.42	0	5,5,5	0.39	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
5	BBI	H	405	-	-	8/18/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAD	H	406	-	-	11/26/62/62	0/5/5/5
5	BBI	A	403	-	-	6/18/22/22	0/3/3/3
7	MCM	C	101	2	-	-	0/2/2/2
8	PEG	H	403	-	-	3/4/4/4	-
7	MCM	D	101	2	-	-	0/2/2/2
6	NAD	A	404	-	-	4/26/62/62	0/5/5/5
8	PEG	H	401	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	BBI	CAM-CAN	-14.20	1.33	1.50
5	H	405	BBI	CAM-CAN	-13.14	1.34	1.50
7	C	101	MCM	C10-C6	-5.92	1.39	1.51
5	A	403	BBI	CAP-CAN	-5.79	1.39	1.49
7	D	101	MCM	C10-C6	-5.72	1.40	1.51
5	H	405	BBI	CAP-CAN	-5.71	1.39	1.49
5	A	403	BBI	CAL-CAG	-4.38	1.33	1.43
5	A	403	BBI	CAK-CAL	-4.18	1.33	1.42
5	H	405	BBI	CAL-CAG	-4.05	1.34	1.43
5	H	405	BBI	CAK-CAL	-3.51	1.35	1.42
6	H	406	NAD	O4B-C1B	2.88	1.45	1.41
6	H	406	NAD	C5A-C4A	2.74	1.48	1.40
6	A	404	NAD	C5A-C4A	2.74	1.48	1.40
6	A	404	NAD	O4D-C1D	2.13	1.44	1.41
6	A	404	NAD	O4B-C1B	2.08	1.44	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	101	MCM	C6-C7-C3	6.94	122.18	118.05
7	D	101	MCM	C6-C7-C3	6.16	121.72	118.05
6	H	406	NAD	C3D-C2D-C1D	4.76	108.14	100.98
5	A	403	BBI	CAT-CAR-IAS	3.61	125.57	119.42
6	A	404	NAD	N3A-C2A-N1A	-3.53	123.16	128.68
6	H	406	NAD	N3A-C2A-N1A	-3.24	123.61	128.68
6	A	404	NAD	C4A-C5A-N7A	-3.22	106.04	109.40
7	C	101	MCM	O1-C3-C2	3.09	119.70	116.03
7	C	101	MCM	O1-C3-C7	-2.99	118.31	121.20
5	A	403	BBI	CAK-CAL-CAG	2.93	122.23	120.38
6	A	404	NAD	PN-O3-PA	-2.92	122.80	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	406	NAD	C4A-C5A-N7A	-2.80	106.48	109.40
5	A	403	BBI	CAT-CBC-IBD	2.71	124.04	119.42
7	D	101	MCM	O1-C3-C2	2.63	119.14	116.03
6	A	404	NAD	C3D-C2D-C1D	2.55	104.82	100.98
7	C	101	MCM	O1-C4-C5	2.40	122.33	119.27
5	A	403	BBI	CAK-CAL-CAM	-2.38	130.76	135.49
5	A	403	BBI	CAL-CAM-CAN	-2.33	120.01	125.12
6	H	406	NAD	C6N-N1N-C2N	-2.30	119.88	121.97
5	A	403	BBI	CAM-CAN-CAP	-2.24	116.39	119.53
5	A	403	BBI	CAQ-CAR-IAS	-2.22	114.51	118.61
6	H	406	NAD	C1B-N9A-C4A	-2.16	122.84	126.64
6	A	404	NAD	C2A-N1A-C6A	2.15	122.44	118.75
5	H	405	BBI	OAO-CAN-CAM	2.08	121.91	119.49
7	D	101	MCM	C8-C7-C6	-2.08	119.69	123.66
7	D	101	MCM	O1-C3-C7	-2.05	119.22	121.20

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	BBI	CAC-CAD-CAE-CAM
5	A	403	BBI	CAL-CAM-CAN-OAO
5	H	405	BBI	CAB-CAC-CAD-CAE
6	A	404	NAD	C5D-O5D-PN-O3
6	H	406	NAD	C5B-O5B-PA-O3
6	H	406	NAD	C2D-C1D-N1N-C2N
6	H	406	NAD	C2D-C1D-N1N-C6N
6	H	406	NAD	C2N-C3N-C7N-O7N
5	H	405	BBI	OAO-CAN-CAP-CBE
5	H	405	BBI	CAM-CAN-CAP-CBE
5	H	405	BBI	CAM-CAN-CAP-CAQ
6	H	406	NAD	C2N-C3N-C7N-N7N
5	H	405	BBI	OAO-CAN-CAP-CAQ
8	H	403	PEG	O1-C1-C2-O2
5	A	403	BBI	CBB-CBA-NAX-CAW
5	H	405	BBI	CAZ-CAY-NAX-CBA
6	H	406	NAD	C4N-C3N-C7N-N7N
8	H	403	PEG	O2-C3-C4-O4
5	A	403	BBI	CAA-CAB-CAC-CAD
6	H	406	NAD	C4N-C3N-C7N-O7N
5	H	405	BBI	CAA-CAB-CAC-CAD
5	A	403	BBI	CBB-CBA-NAX-CAY

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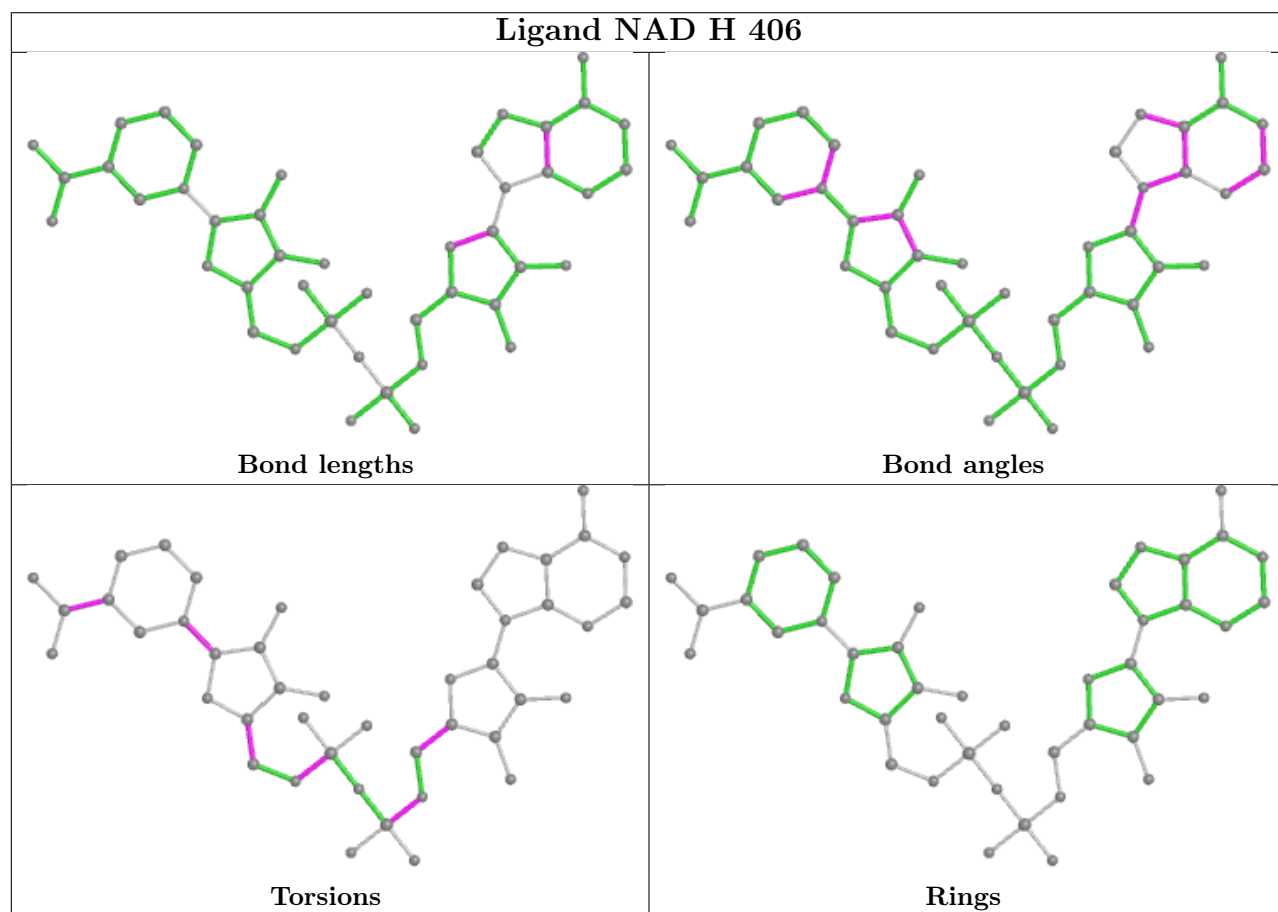
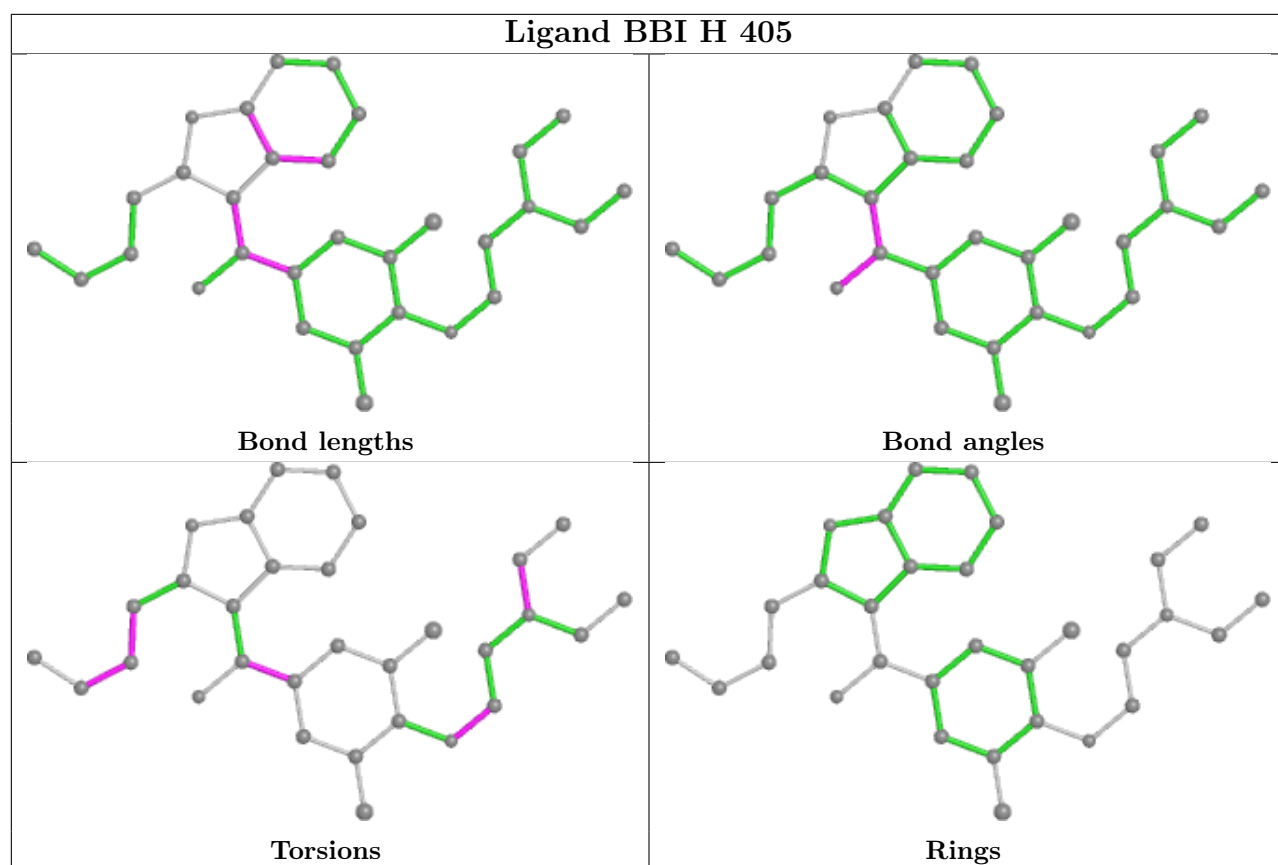
Mol	Chain	Res	Type	Atoms
8	H	401	PEG	O1-C1-C2-O2
8	H	401	PEG	O2-C3-C4-O4
8	H	403	PEG	C4-C3-O2-C2
6	H	406	NAD	C5D-O5D-PN-O3
5	H	405	BBI	CAW-CAV-OAU-CAT
6	A	404	NAD	O4D-C4D-C5D-O5D
6	H	406	NAD	O4B-C4B-C5B-O5B
5	A	403	BBI	CAW-CAV-OAU-CAT
6	A	404	NAD	O4B-C4B-C5B-O5B
6	H	406	NAD	O4D-C4D-C5D-O5D
6	A	404	NAD	C5D-O5D-PN-O1N
6	H	406	NAD	C5B-O5B-PA-O1A

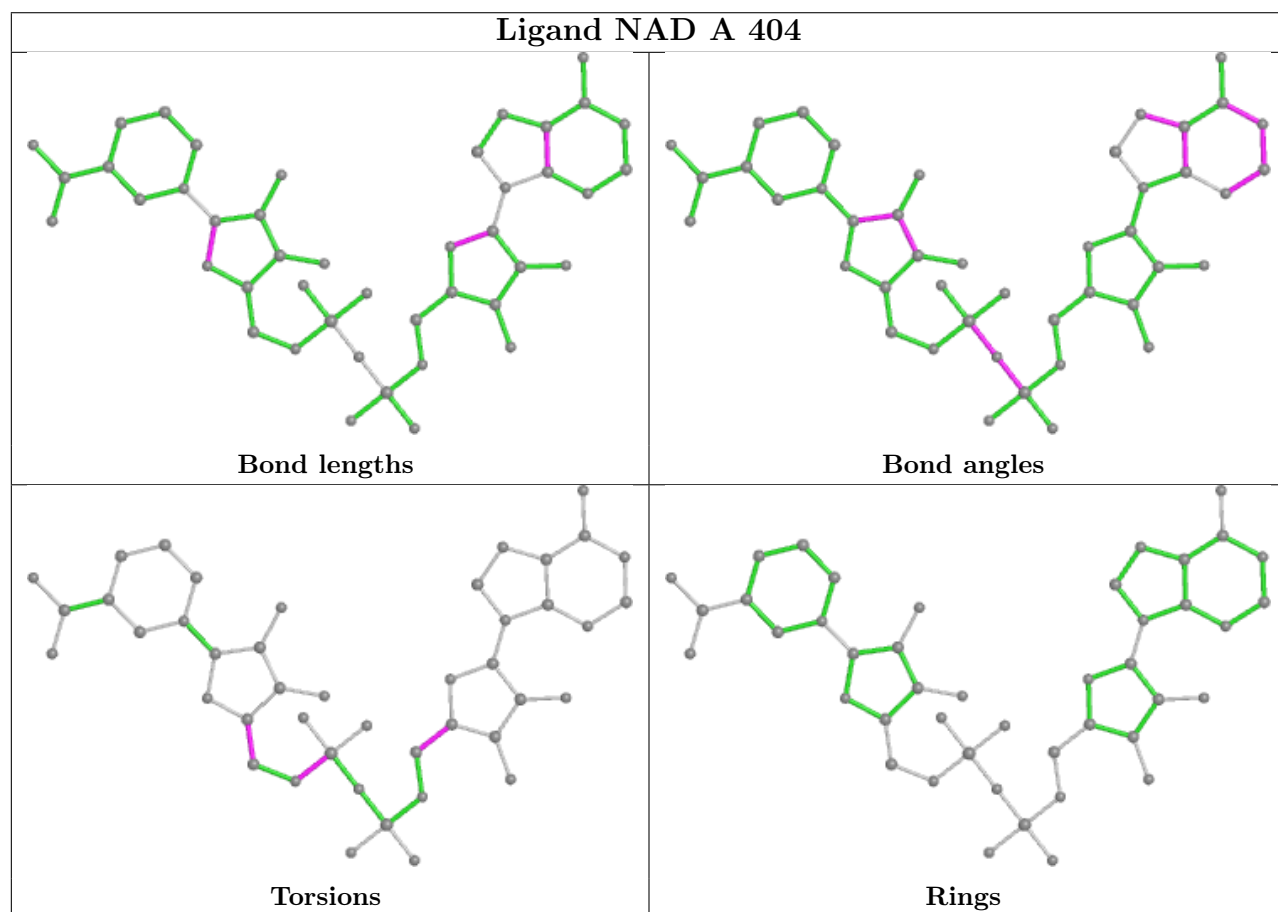
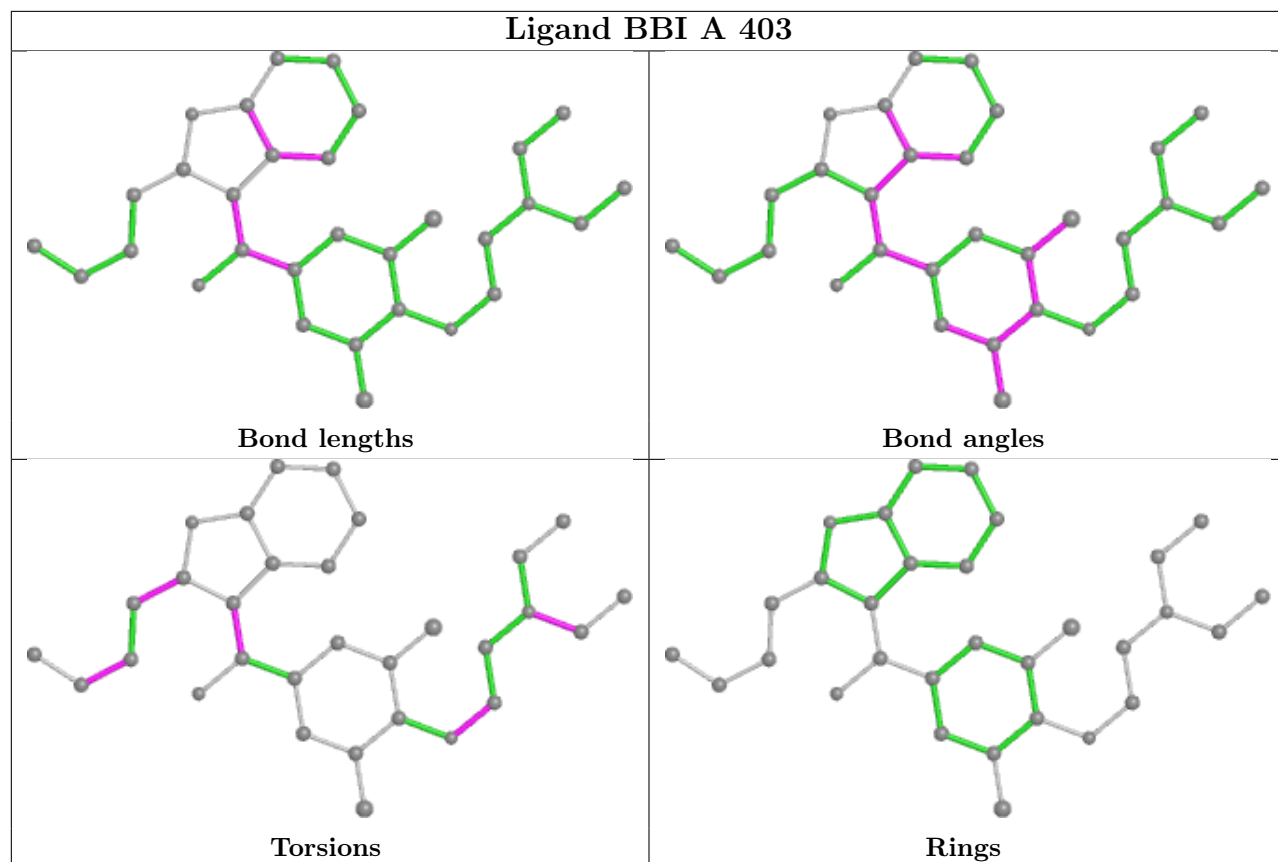
There are no ring outliers.

7 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	405	BBI	14	0
6	H	406	NAD	10	0
5	A	403	BBI	6	1
7	C	101	MCM	3	0
7	D	101	MCM	3	0
6	A	404	NAD	2	0
8	H	401	PEG	8	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	271/271 (100%)	-0.02	8 (2%) 50 36	14, 31, 105, 122	0
1	H	271/271 (100%)	-0.05	8 (2%) 50 36	13, 29, 67, 108	0
2	C	3/4 (75%)	0.08	0 100 100	37, 37, 43, 48	0
2	D	3/4 (75%)	-0.23	0 100 100	35, 35, 40, 52	0
All	All	548/550 (99%)	-0.03	16 (2%) 51 37	13, 30, 79, 122	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	GLY	8.3
1	A	172	ASP	6.2
1	H	163	GLY	5.0
1	H	167	ASN	4.2
1	A	167	ASN	4.1
1	A	166	SER	3.7
1	H	162	SER	3.1
1	H	166	SER	3.1
1	A	157	PHE	3.0
1	A	169	GLN	2.7
1	H	121	GLY	2.7
1	H	327	PHE	2.7
1	A	170	GLN	2.3
1	H	161	GLY	2.1
1	A	156	ASP	2.1
1	H	172	ASP	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	ALY	C	4	12/13	0.95	0.26	27,30,31,31	0
2	ALY	D	4	12/13	0.97	0.21	24,25,27,27	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

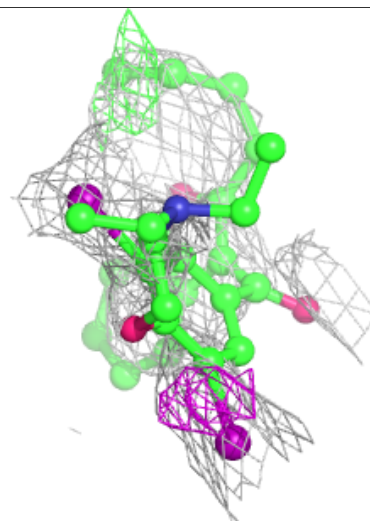
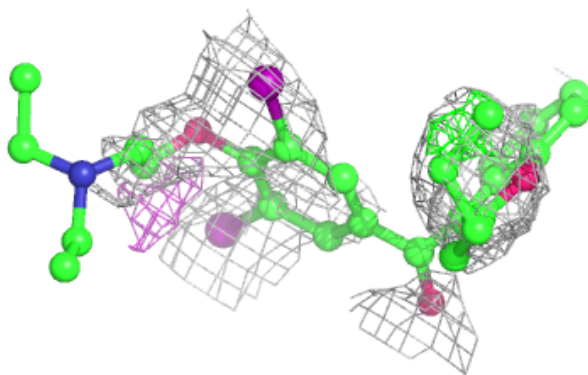
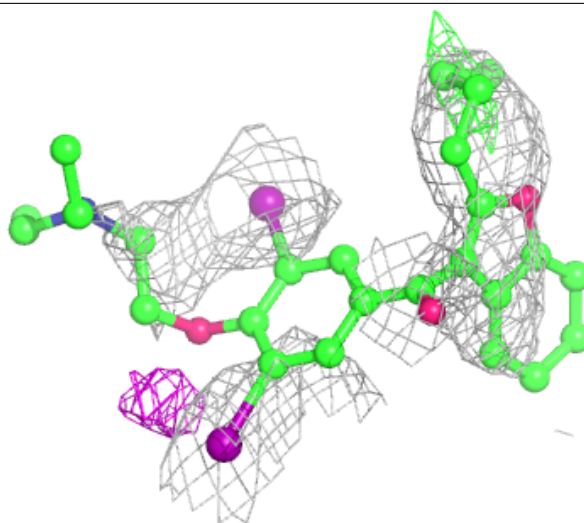
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	BBI	A	403	31/31	0.73	0.43	88,124,178,212	0
5	BBI	H	405	31/31	0.79	0.45	81,108,155,189	0
6	NAD	A	404	44/44	0.79	0.56	77,101,112,117	0
6	NAD	H	406	44/44	0.84	0.35	62,68,73,74	0
8	PEG	H	403	7/7	0.88	0.25	33,34,36,36	0
8	PEG	H	401	7/7	0.90	0.27	20,20,21,22	0
4	MG	H	404	1/1	0.90	0.23	2,2,2,2	0
7	MCM	C	101	13/13	0.93	0.20	26,26,28,28	0
7	MCM	D	101	13/13	0.94	0.22	21,22,23,23	0
4	MG	A	402	1/1	0.94	0.13	2,2,2,2	0
3	ZN	A	401	1/1	0.99	0.10	28,28,28,28	0
3	ZN	H	402	1/1	0.99	0.06	29,29,29,29	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.

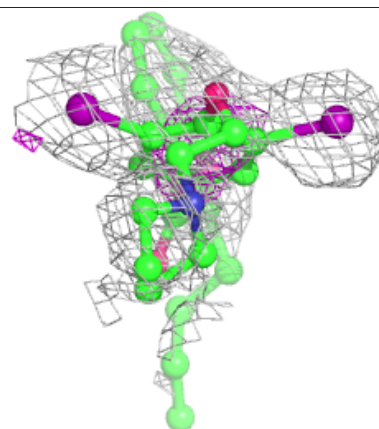
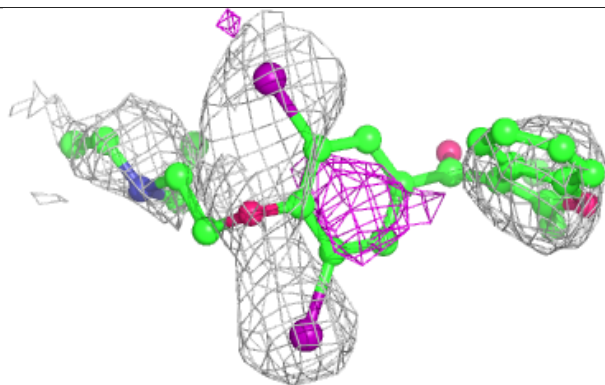
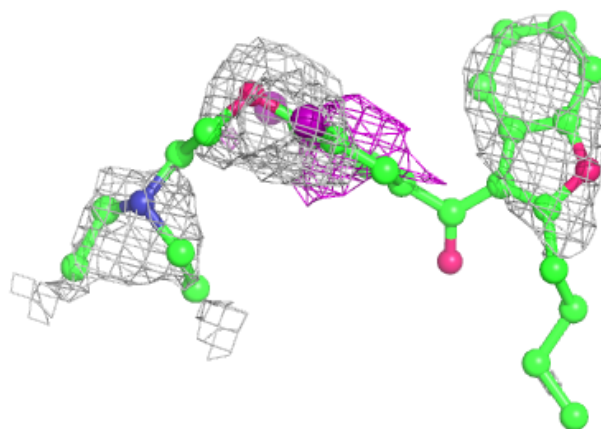
**Electron density around BBI A 403:**

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

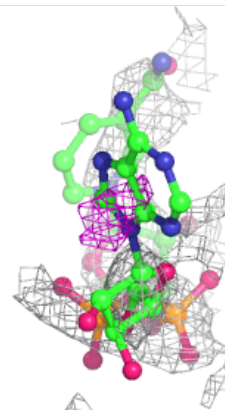
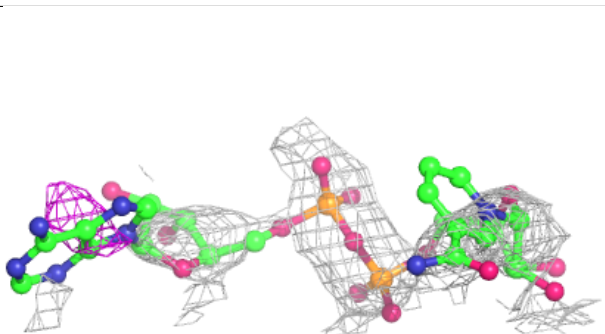
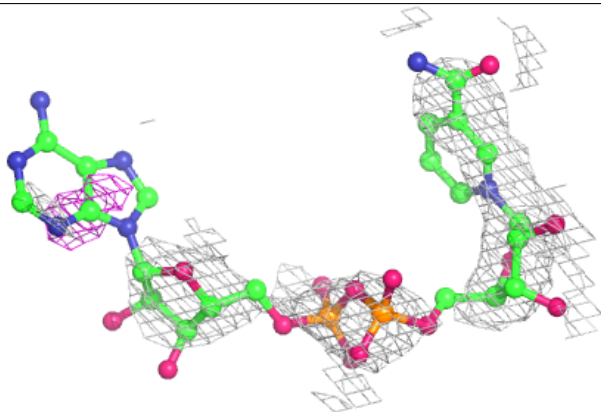


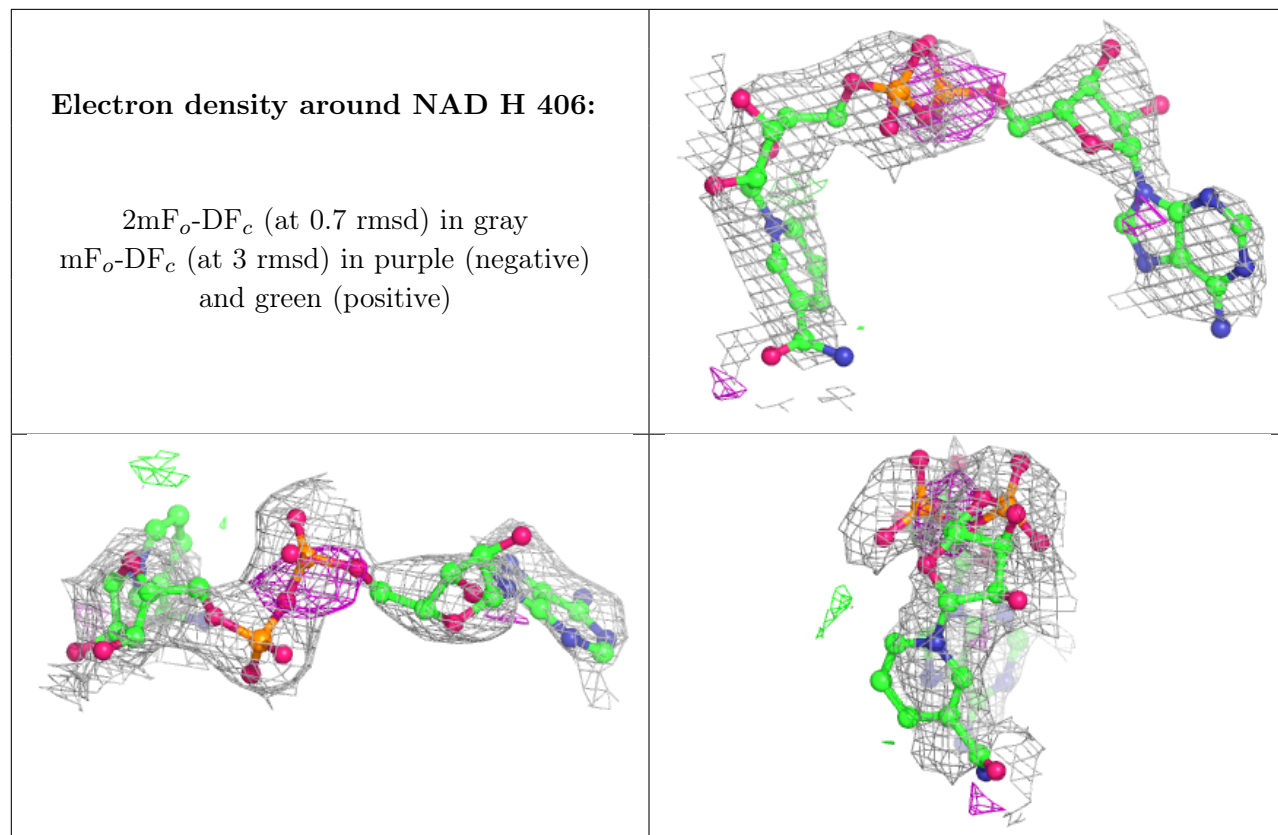
**Electron density around BBI H 405:**

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

**Electron density around NAD A 404:**

$2mF_o-DF_c$  (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.