



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:28 PM UTC

PDB ID : 9HI1 / pdb\_00009hi1  
Title : STRUCTURE OF HUMAN UDP-GALACTOSE 4-EPIMERASE IN COM-  
PLEX WITH COMPOUND WBX09  
Authors : Mouilleron, S.; Schumann, B.; Browne, W.; Purkiss, A.; Weckwerth, T.;  
Ogrodowicz, R.; Prema, R.; Kunzelmann, S.; Roustan, C.  
Deposited on : 2024-11-22  
Resolution : 0.95 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

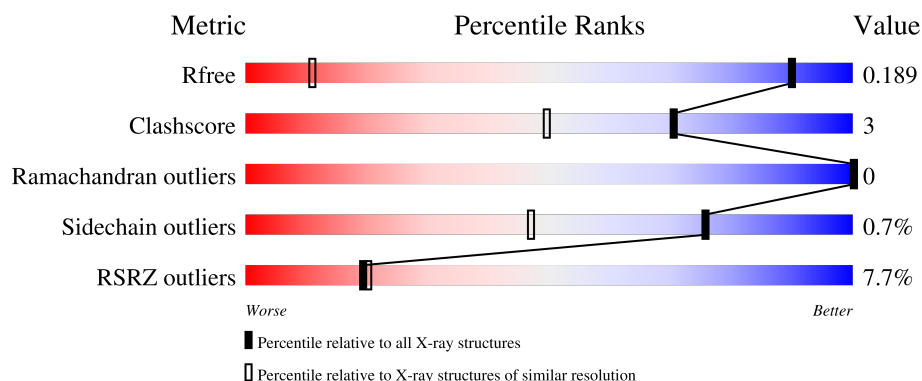
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 0.95 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))
$R_{free}$	180053	1045 (1.00-0.92)
Clashscore	190562	1090 (1.00-0.92)
Ramachandran outliers	187476	1032 (1.00-0.92)
Sidechain outliers	187428	1033 (1.00-0.92)
RSRZ outliers	180081	1043 (1.00-0.92)

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	344	<div> <div>9%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	344	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>9%</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
2	EDO	B	405	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6341 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 UDP-glucose 4-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	343	Total	C	N	O	S	0	30	0
			2841	1808	492	520	21			
1	A	344	Total	C	N	O	S	0	17	0
			2735	1749	467	501	18			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



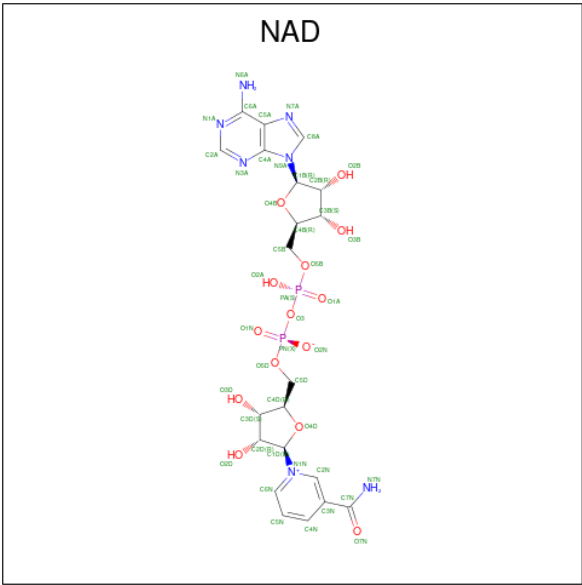
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

Continued from previous page...

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

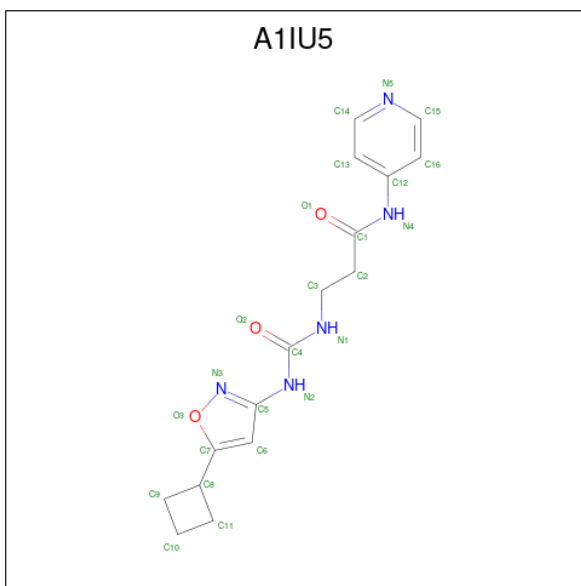
- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 4 is 3-[(5-cyclobutyl-1,2-oxazol-3-yl)carbamoylamino]- {N}-pyridin-4-yl-propanami

de (CCD ID: A1IU5) (formula: C<sub>16</sub>H<sub>19</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			24	16	5	3		
4	A	1	Total	C	N	O	0	0
			24	16	5	3		

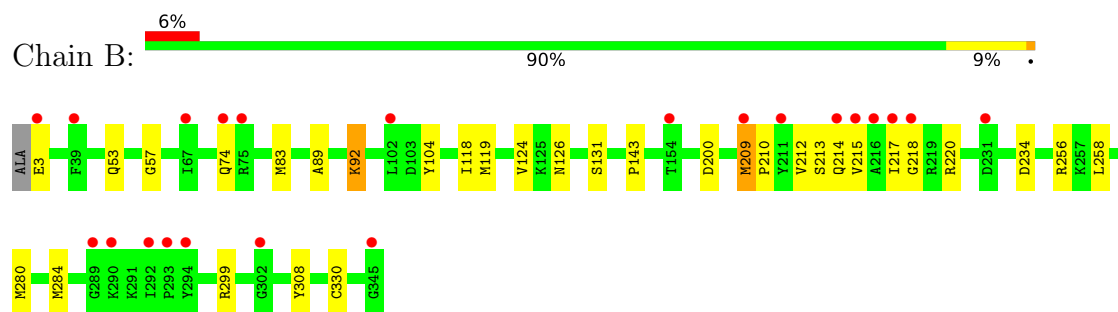
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	301	Total	O	0	2
			301	301		
5	A	280	Total	O	0	2
			280	280		

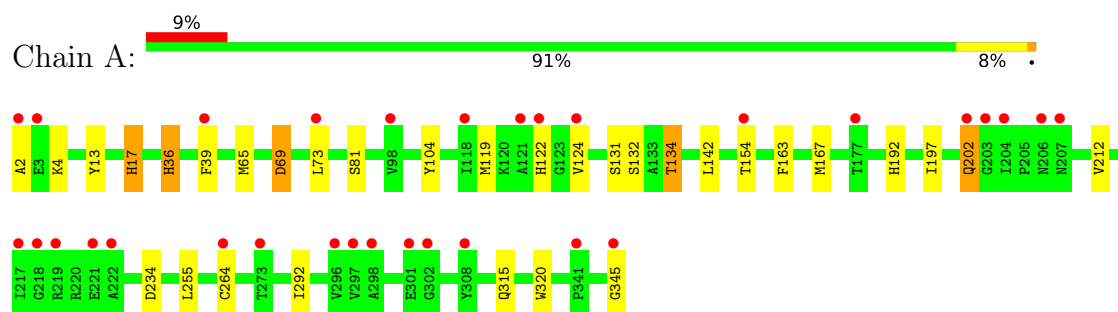
### 3 Residue-property plots

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: UDP-glucose 4-epimerase



- Molecule 1: UDP-glucose 4-epimerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.15Å 110.20Å 135.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.76 – 0.95 57.76 – 0.95	Depositor EDS
% Data completeness (in resolution range)	94.5 (57.76-0.95) 94.5 (57.76-0.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 0.95Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, $R_{free}$	0.181 , 0.189 0.181 , 0.189	Depositor DCC
$R_{free}$ test set	2000 reflections (0.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.6	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 27.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6341	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% 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: NAD, EDO, A1IU5

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	0/2842	1.06	13/3844 (0.3%)
1	B	0.72	0/2955	1.01	4/3995 (0.1%)
All	All	0.72	0/5797	1.03	17/7839 (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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	CB-CG-CD2	-8.54	120.09	131.20
1	A	122	HIS	CB-CG-CD2	-7.87	120.97	131.20
1	A	36	HIS	CB-CG-ND1	6.78	132.87	122.70
1	A	122	HIS	CB-CG-ND1	6.49	132.43	122.70
1	A	202	GLN	CB-CA-C	6.24	120.64	110.22
1	A	4	LYS	CB-CG-CD	-5.76	98.04	111.30
1	A	17	HIS	CB-CG-ND1	5.76	131.35	122.70
1	A	17	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	299	ARG	CB-CA-C	-5.50	99.77	109.62
1	B	299	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	A	154	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	142	LEU	O-C-N	-5.34	118.09	121.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	234	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	69[A]	ASP	CB-CA-C	-5.21	102.45	111.30
1	A	69[B]	ASP	CB-CA-C	-5.21	102.45	111.30
1	A	234	ASP	CA-CB-CG	5.16	117.76	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	TYR	Sidechain
1	B	104	TYR	Sidechain
1	B	256	ARG	Sidechain

## 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	2735	0	2734	18	0
1	B	2841	0	2841	21	0
2	A	28	0	42	1	0
2	B	20	0	28	3	0
3	A	44	0	26	1	0
3	B	44	0	26	1	0
4	A	24	0	0	0	0
4	B	24	0	0	0	0
5	A	280	0	0	2	0
5	B	301	0	0	1	0
All	All	6341	0	5697	39	0

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

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209[A]:MET:HA	1:B:209[A]:MET:HE2	1.61	0.82
1:A:17:HIS:HE1	1:A:192:HIS:H	1.29	0.80
1:B:210[A]:PRO:O	1:B:213[A]:SER:N	2.17	0.77
1:B:53:GLN:HB3	2:B:403:EDO:H22	1.79	0.65
1:B:3:GLU:OE1	1:B:83[B]:MET:HB3	2.00	0.62
1:B:212[B]:VAL:HG12	1:B:284[B]:MET:HG2	1.85	0.59
1:A:119:MET:HB3	1:A:124:VAL:O	2.03	0.58
1:A:17:HIS:CE1	1:A:192:HIS:H	2.16	0.58
1:A:36:HIS:HE1	5:A:575:HOH:O	1.88	0.57
1:A:39[B]:PHE:CZ	1:A:345:GLY:HA3	2.40	0.57
1:A:132:SER:OG	1:A:134[A]:THR:HG22	2.08	0.54
1:A:212:VAL:HG13	1:A:292:ILE:HD13	1.91	0.53
1:A:13:TYR:O	1:A:17:HIS:HD2	1.92	0.53
1:B:210[A]:PRO:O	1:B:214[A]:GLN:N	2.40	0.53
1:B:209[A]:MET:SD	1:B:280:MET:HE3	2.49	0.52
1:A:255:LEU:CD1	2:A:406:EDO:H22	2.40	0.51
1:A:2:ALA:HA	1:A:81[B]:SER:HB3	1.93	0.51
1:B:74[A]:GLN:HG2	1:B:118:ILE:HD12	1.92	0.51
1:A:197:ILE:O	5:A:501:HOH:O	2.19	0.49
1:B:131:SER:O	3:B:406:NAD:H6N	2.12	0.49
1:A:39[A]:PHE:CZ	1:A:202:GLN:HG2	2.48	0.49
1:B:215[A]:VAL:O	1:B:218:GLY:N	2.45	0.49
1:B:284[A]:MET:HE2	1:B:330:CYS:SG	2.54	0.47
1:B:214[B]:GLN:HA	1:B:217:ILE:HG12	1.96	0.47
1:A:131:SER:O	3:A:408:NAD:H6N	2.14	0.47
1:B:215[A]:VAL:HG22	1:B:220:ARG:HB2	1.99	0.45
1:A:163:PHE:O	1:A:167[A]:MET:HG3	2.16	0.45
1:A:315:GLN:HA	1:A:320:TRP:O	2.18	0.44
1:B:119:MET:HB3	1:B:124:VAL:O	2.18	0.43
1:B:126:ASN:HB3	1:B:258:LEU:HD13	2.02	0.41
1:B:284[A]:MET:HE2	1:B:284[A]:MET:HB2	1.66	0.41
1:B:92[C]:LYS:HE3	5:B:531:HOH:O	2.20	0.41
1:B:143:PRO:HB3	1:B:308:TYR:CE2	2.56	0.41
1:A:65:MET:HE1	1:A:73:LEU:HD13	2.02	0.41
1:B:57:GLY:C	2:B:403:EDO:H21	2.46	0.41
1:B:89:ALA:O	2:B:405:EDO:H11	2.21	0.41
1:B:213[B]:SER:HA	1:B:284[B]:MET:HE2	2.02	0.40
1:A:65:MET:CE	1:A:73:LEU:HD13	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	360/344 (105%)	352 (98%)	8 (2%)	0	100	100
1	B	373/344 (108%)	366 (98%)	7 (2%)	0	100	100
All	All	733/688 (106%)	718 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	289/278 (104%)	286 (99%)	3 (1%)	68	34
1	B	302/278 (109%)	297 (98%)	5 (2%)	53	18
All	All	591/556 (106%)	583 (99%)	8 (1%)	76	21

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92[A]	LYS
1	B	92[B]	LYS
1	B	92[C]	LYS
1	B	209[A]	MET
1	B	209[B]	MET
1	A	134[A]	THR
1	A	134[B]	THR
1	A	264	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	GLN
1	A	17	HIS
1	A	36	HIS
1	A	122	HIS
1	A	187	ASN
1	A	206	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
2	EDO	A	402	-	3,3,3	0.52	0	2,2,2	0.17	0
4	A1IU5	A	409	-	25,26,26	0.46	0	31,34,34	0.83	1 (3%)
3	NAD	B	406	-	46,48,48	0.77	1 (2%)	64,73,73	1.12	5 (7%)
2	EDO	A	405	-	3,3,3	0.09	0	2,2,2	0.29	0
2	EDO	A	406	-	3,3,3	0.10	0	2,2,2	0.58	0
2	EDO	A	407	-	3,3,3	0.10	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	EDO	A	401	-	3,3,3	0.33	0	2,2,2	0.44	0
2	EDO	A	403	-	3,3,3	0.29	0	2,2,2	0.49	0
2	EDO	B	403	-	3,3,3	0.10	0	2,2,2	0.11	0
3	NAD	A	408	-	46,48,48	0.71	0	64,73,73	1.10	4 (6%)
2	EDO	B	404	-	3,3,3	0.65	0	2,2,2	1.11	0
4	A1IU5	B	407	-	25,26,26	0.65	0	31,34,34	1.09	2 (6%)
2	EDO	A	404	-	3,3,3	0.13	0	2,2,2	0.30	0
2	EDO	B	401	-	3,3,3	0.50	0	2,2,2	0.17	0
2	EDO	B	402	-	3,3,3	0.69	0	2,2,2	0.46	0
2	EDO	B	405	-	3,3,3	2.33	2 (66%)	2,2,2	2.00	1 (50%)

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	EDO	A	402	-	-	0/1/1/1	-
4	A1IU5	A	409	-	-	1/16/24/24	0/3/3/3
3	NAD	B	406	-	-	3/30/62/62	0/5/5/5
2	EDO	A	405	-	-	1/1/1/1	-
2	EDO	A	406	-	-	1/1/1/1	-
2	EDO	A	407	-	-	1/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	B	403	-	-	1/1/1/1	-
3	NAD	A	408	-	-	3/30/62/62	0/5/5/5
2	EDO	B	404	-	-	0/1/1/1	-
4	A1IU5	B	407	-	-	1/16/24/24	0/3/3/3
2	EDO	A	404	-	-	1/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	B	405	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	405	EDO	O2-C2	-2.60	1.28	1.42
2	B	405	EDO	O1-C1	2.41	1.54	1.42
3	B	406	NAD	C2N-N1N	2.34	1.37	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	407	A1IU5	C9-C8-C7	-4.73	110.85	119.02
3	B	406	NAD	C5D-C4D-C3D	3.57	128.07	115.21
3	A	408	NAD	C5D-C4D-C3D	3.26	126.94	115.21
3	A	408	NAD	O2N-PN-O5D	2.99	121.14	107.57
3	B	406	NAD	O2N-PN-O5D	2.93	120.85	107.57
3	B	406	NAD	C3N-C7N-N7N	2.64	120.99	117.74
4	A	409	A1IU5	C9-C8-C7	-2.51	114.69	119.02
4	B	407	A1IU5	N2-C5-N3	-2.27	116.47	123.52
3	B	406	NAD	O3-PN-O1N	-2.27	103.88	110.70
3	A	408	NAD	C6N-N1N-C2N	-2.15	120.05	121.88
2	B	405	EDO	O1-C1-C2	2.13	128.57	112.39
3	A	408	NAD	O3-PN-O1N	-2.09	104.41	110.70
3	B	406	NAD	C4D-O4D-C1D	2.05	111.80	109.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	407	A1IU5	C6-C7-C8-C11
2	B	403	EDO	O1-C1-C2-O2
2	A	404	EDO	O1-C1-C2-O2
2	A	406	EDO	O1-C1-C2-O2
2	A	407	EDO	O1-C1-C2-O2
3	B	406	NAD	PN-O3-PA-O5B
3	A	408	NAD	PN-O3-PA-O5B
3	A	408	NAD	PA-O3-PN-O2N
3	B	406	NAD	PA-O3-PN-O2N
2	A	405	EDO	O1-C1-C2-O2
4	A	409	A1IU5	C6-C7-C8-C11
2	B	405	EDO	O1-C1-C2-O2
3	A	408	NAD	O4B-C4B-C5B-O5B
2	A	401	EDO	O1-C1-C2-O2
3	B	406	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

5 monomers are involved in 6 short contacts:

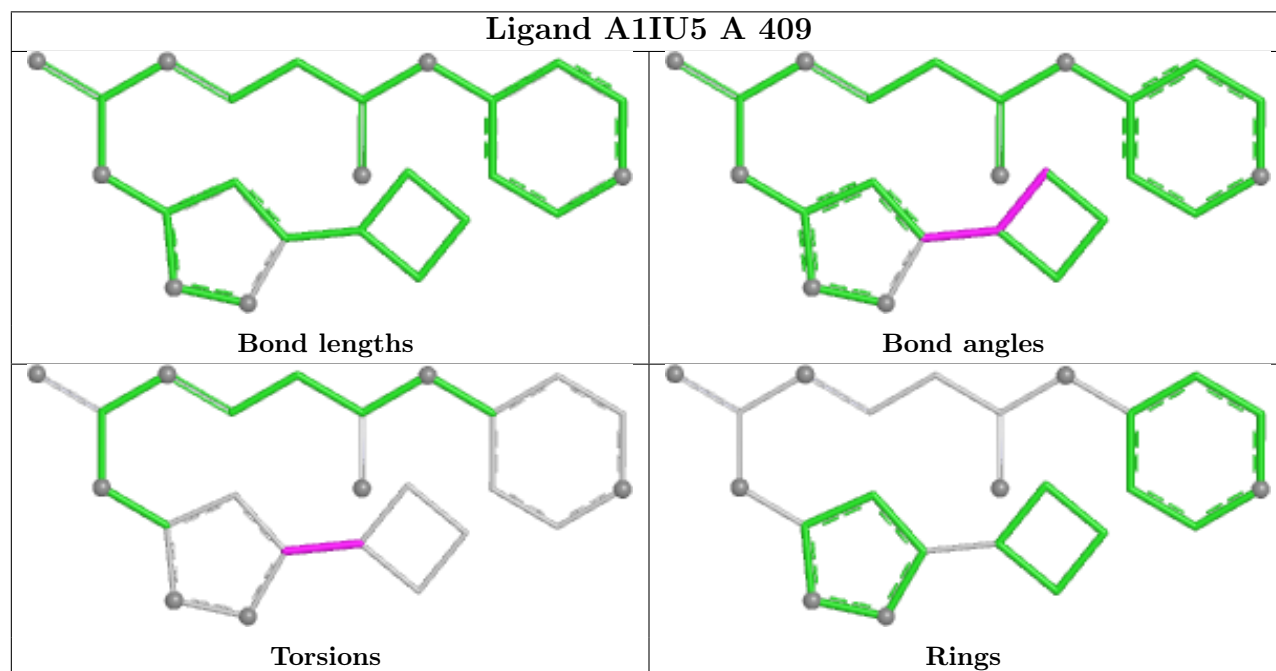
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	NAD	1	0
2	A	406	EDO	1	0

*Continued on next page...*

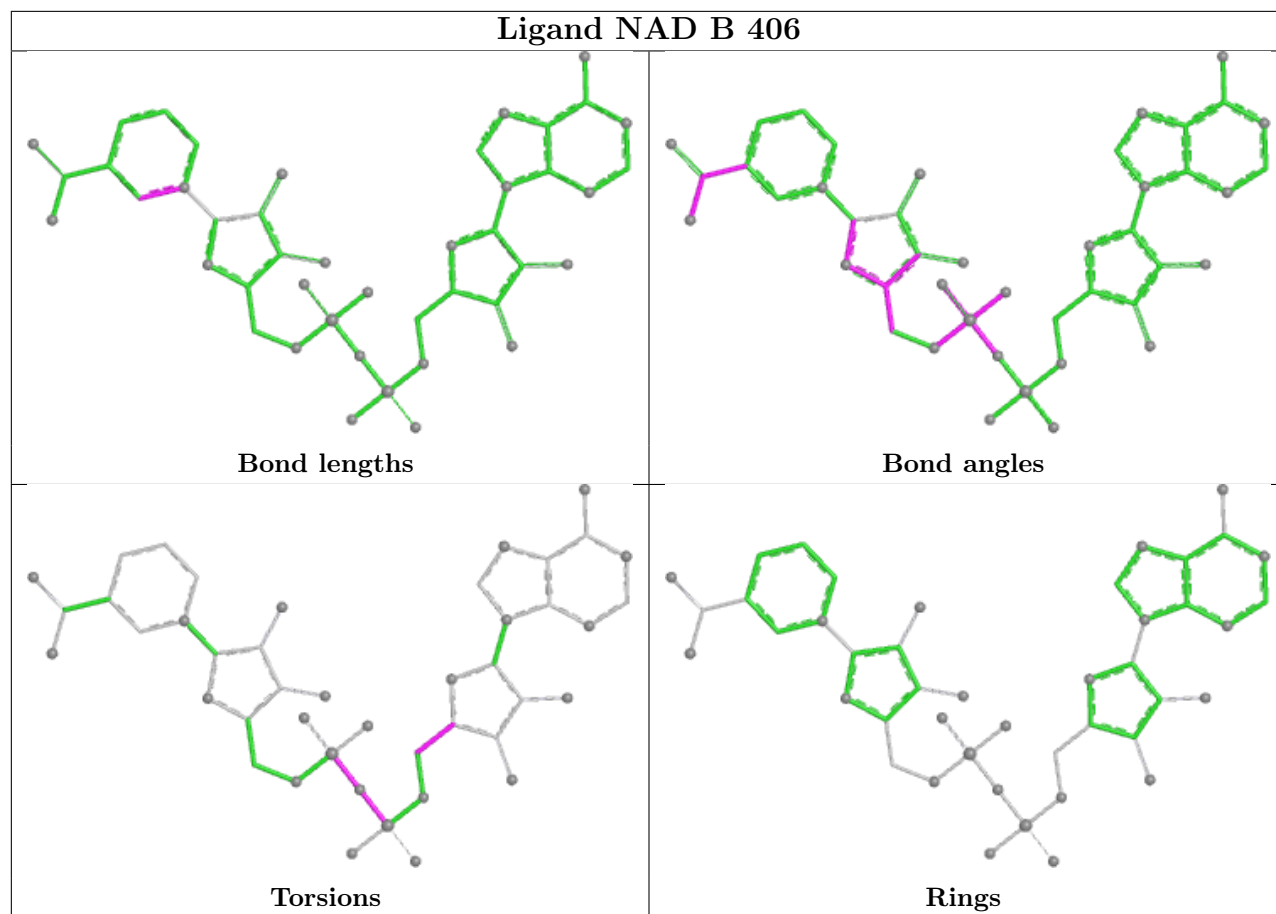
Continued from previous page...

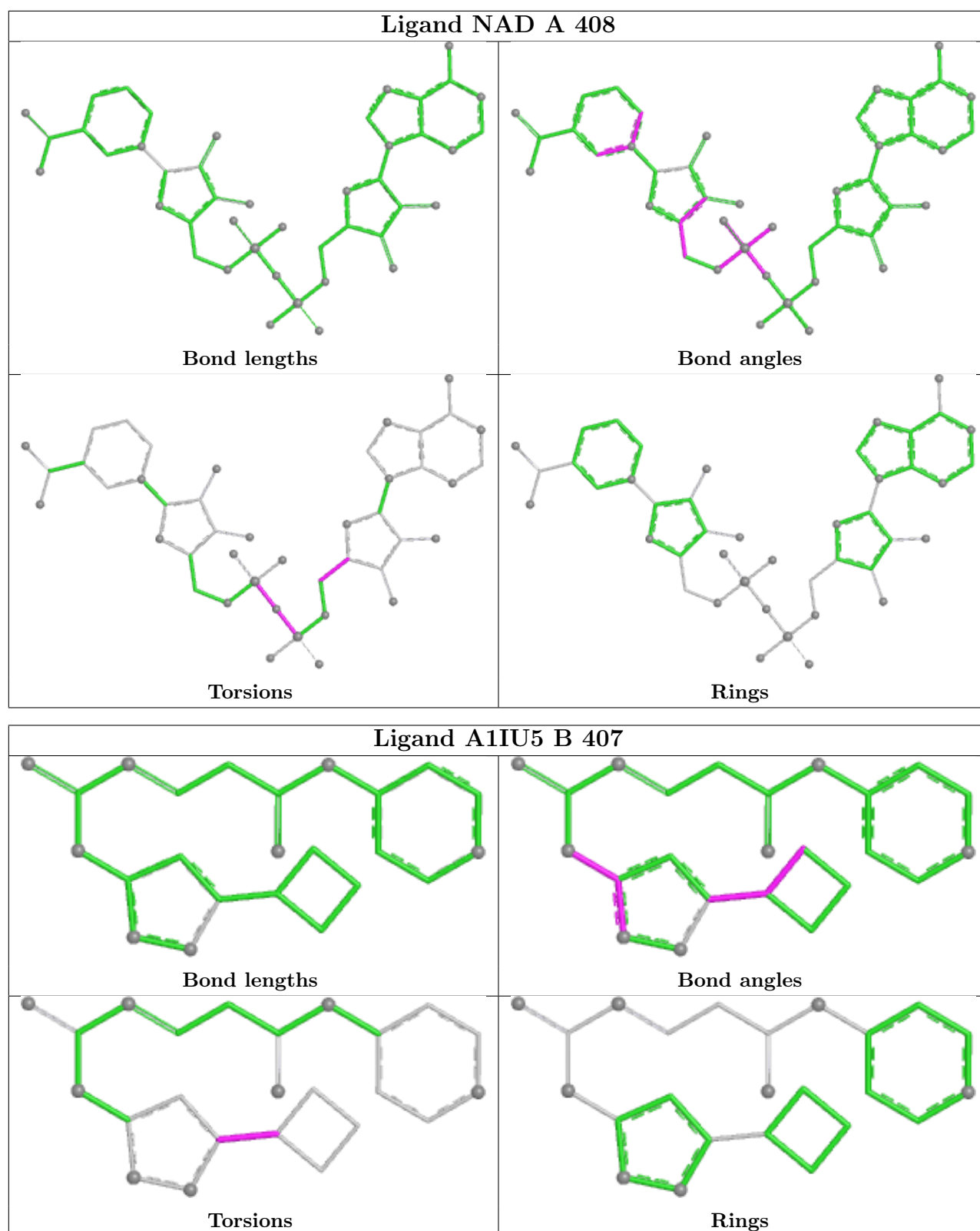
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	EDO	2	0
3	A	408	NAD	1	0
2	B	405	EDO	1	0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	344/344 (100%)	0.75	31 (9%)	15 14	6, 13, 26, 37	17 (4%)
1	B	343/344 (99%)	0.55	22 (6%)	25 27	4, 11, 21, 40	30 (8%)
All	All	687/688 (99%)	0.65	53 (7%)	19 20	4, 12, 24, 40	47 (6%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	CYS	7.1
1	B	217	ILE	6.3
1	A	204	ILE	5.3
1	B	154[A]	THR	5.2
1	A	222	ALA	4.9
1	A	2	ALA	4.7
1	A	118	ILE	4.6
1	A	345	GLY	4.3
1	B	215[A]	VAL	3.9
1	B	218	GLY	3.9
1	A	302	GLY	3.9
1	B	345	GLY	3.5
1	A	221	GLU	3.5
1	B	289	GLY	3.4
1	B	216	ALA	3.4
1	A	121	ALA	3.4
1	B	39	PHE	3.3
1	A	218	GLY	3.3
1	A	301	GLU	3.3
1	A	297	VAL	3.3
1	A	206	ASN	3.2
1	A	217	ILE	3.1
1	A	154	THR	3.0
1	B	211[A]	TYR	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	124	VAL	2.9
1	A	202	GLN	2.8
1	B	74[A]	GLN	2.8
1	A	219	ARG	2.8
1	A	298	ALA	2.7
1	B	294	TYR	2.7
1	B	231	ASP	2.7
1	B	302	GLY	2.6
1	A	177	THR	2.6
1	A	98	VAL	2.5
1	A	3	GLU	2.5
1	B	75[A]	ARG	2.5
1	A	39[A]	PHE	2.5
1	A	122	HIS	2.4
1	B	102	LEU	2.4
1	B	290	LYS	2.3
1	A	296	VAL	2.3
1	B	67	ILE	2.3
1	A	273	THR	2.3
1	B	292	ILE	2.2
1	B	209[A]	MET	2.2
1	B	293	PRO	2.2
1	A	203	GLY	2.2
1	B	214[A]	GLN	2.2
1	A	341	PRO	2.1
1	A	207	ASN	2.1
1	A	73	LEU	2.0
1	B	3	GLU	2.0
1	A	308	TYR	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 oligosaccharides in this entry.

## 6.4 Ligands ⓘ

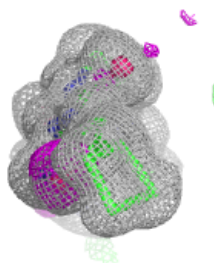
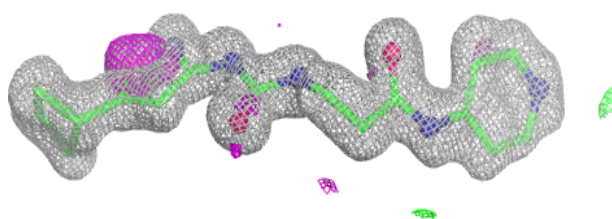
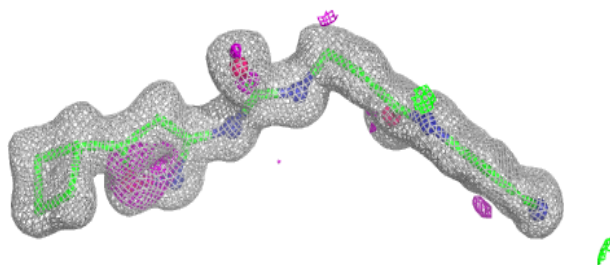
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	EDO	A	404	4/4	0.54	0.31	46,61,62,64	0
2	EDO	A	405	4/4	0.80	0.21	45,48,50,54	0
2	EDO	A	401	4/4	0.82	0.14	22,23,28,31	0
2	EDO	B	403	4/4	0.86	0.14	23,35,36,43	0
2	EDO	A	406	4/4	0.86	0.14	23,28,33,40	0
2	EDO	A	407	4/4	0.87	0.13	31,36,36,44	0
2	EDO	B	404	4/4	0.88	0.12	18,25,26,36	0
2	EDO	A	403	4/4	0.92	0.09	20,21,21,21	0
2	EDO	B	405	4/4	0.93	0.11	12,12,22,25	0
4	A1IU5	B	407	24/24	0.94	0.09	13,17,27,29	0
4	A1IU5	A	409	24/24	0.94	0.10	16,18,32,33	0
2	EDO	B	402	4/4	0.95	0.08	15,16,17,18	0
2	EDO	B	401	4/4	0.95	0.08	14,15,16,17	0
2	EDO	A	402	4/4	0.97	0.07	15,16,16,17	0
3	NAD	A	408	44/44	0.98	0.06	8,10,16,18	0
3	NAD	B	406	44/44	0.99	0.05	7,9,12,14	0

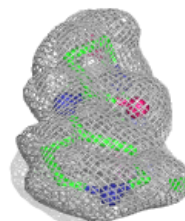
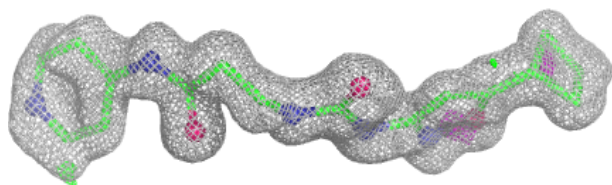
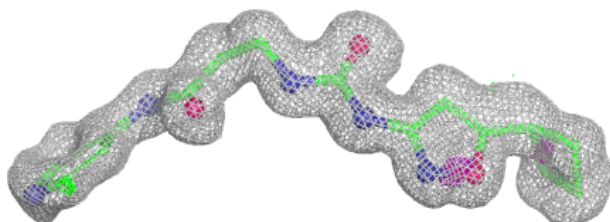
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1IU5 B 407:**

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

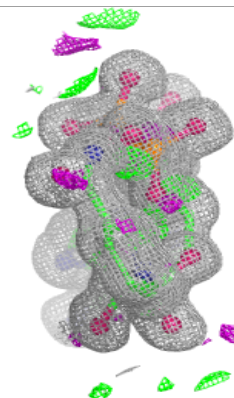
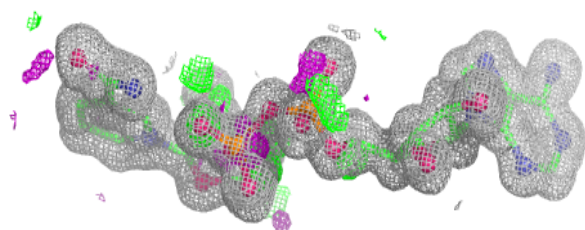
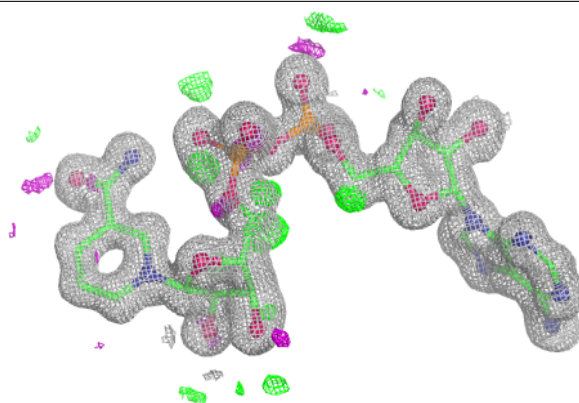
**Electron density around A1IU5 A 409:**

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

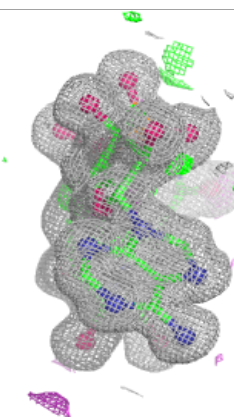
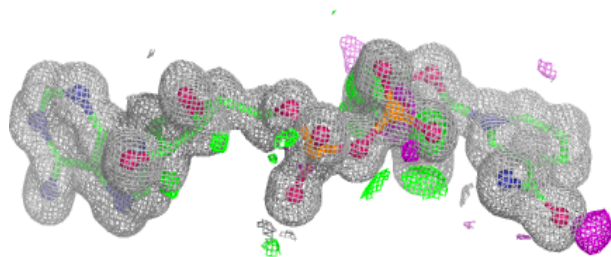
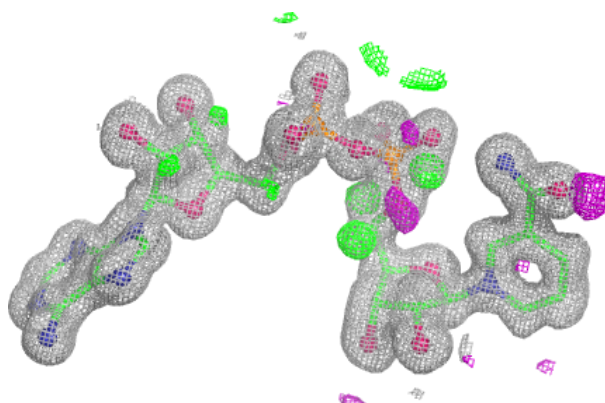


**Electron density around NAD A 408:**

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

**Electron density around NAD B 406:**

$2mF_o-DF_c$  (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.