



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 02:58 PM EDT

PDB ID : 6IHE
Title : Crystal structure of Malate dehydrogenase from Metallosphaera sedula
Authors : Lee, D.; Kim, K.J.
Deposited on : 2018-09-29
Resolution : 1.90 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

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

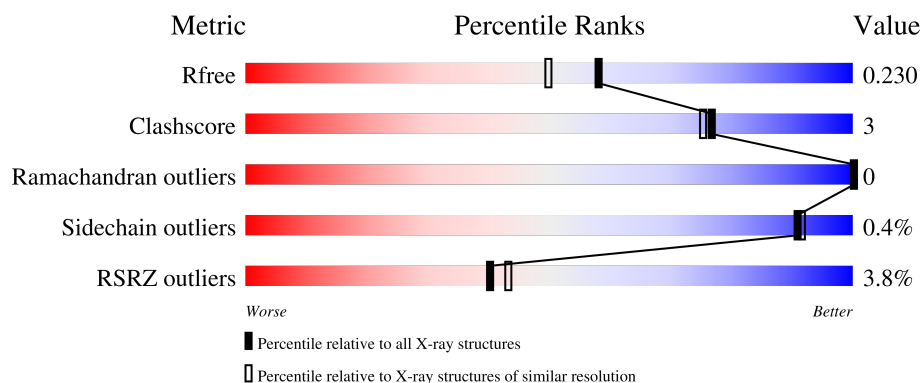
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

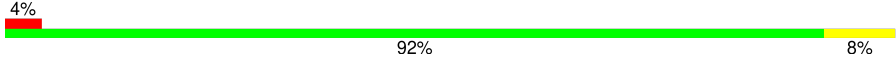
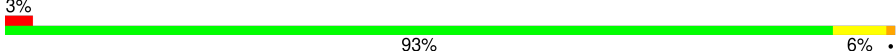
The reported resolution of this entry is 1.90 Å.

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 ≥ 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	303	
1	B	303	

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	MLT	A	402	-	X	-	-
3	MLT	B	402	-	X	-	-
4	GOL	B	403	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5098 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 Malate dehydrogenase (NAD).

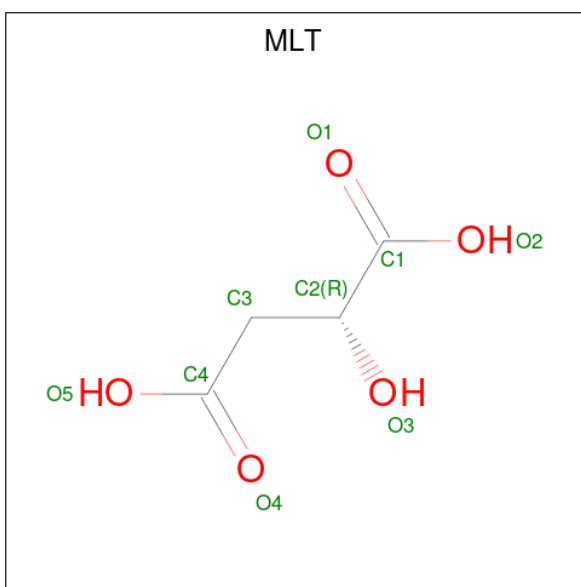
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2326	1487	387	441	11			
1	B	303	Total	C	N	O	S	0	0	0
			2326	1487	387	441	11			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



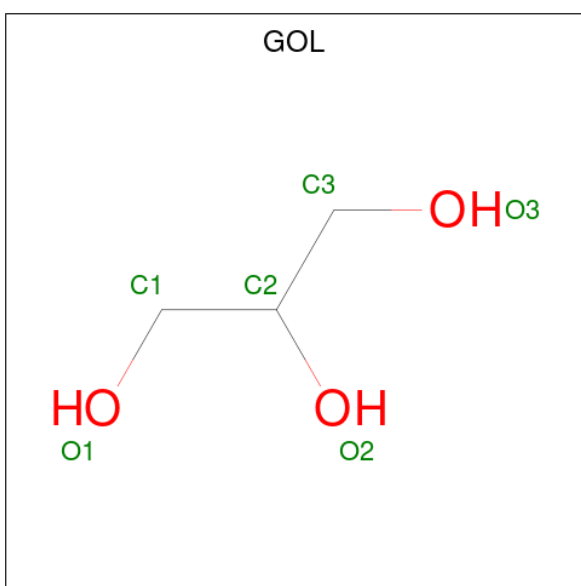
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



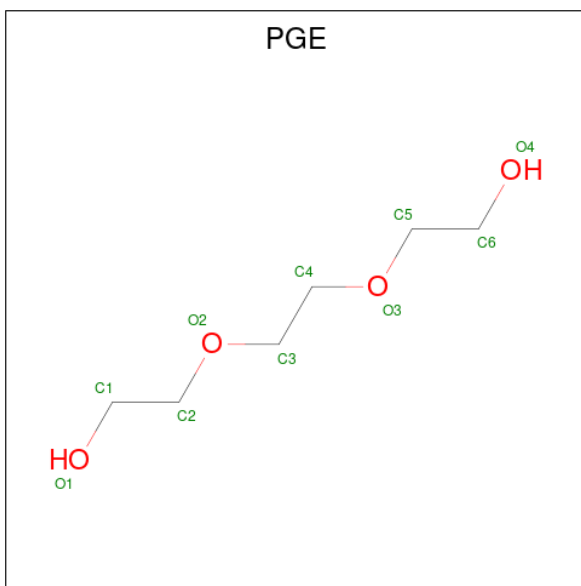
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		
3	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



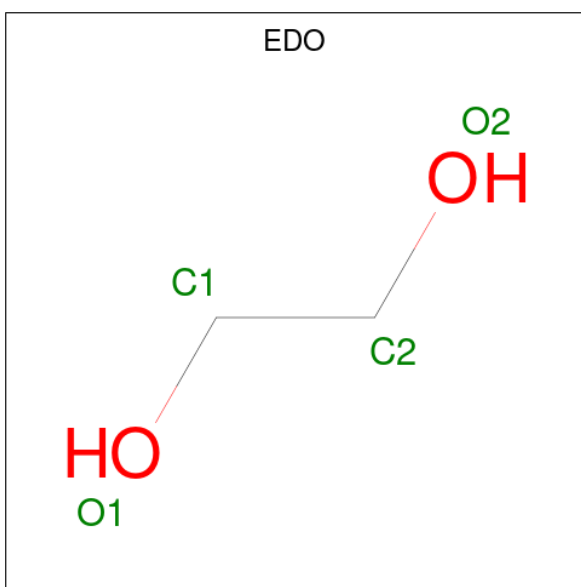
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



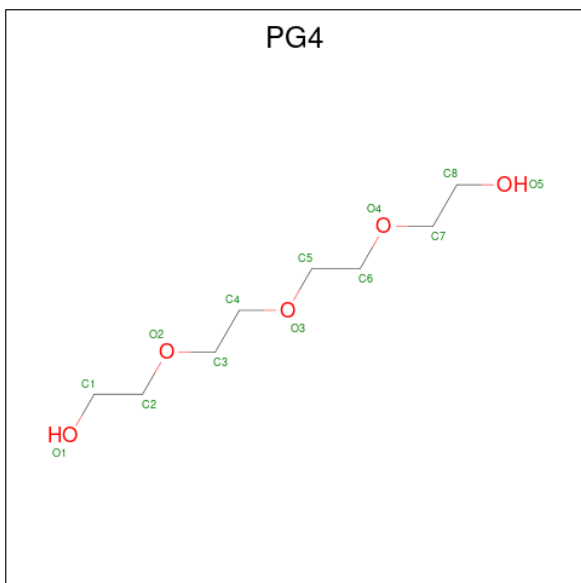
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			9	6	3		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



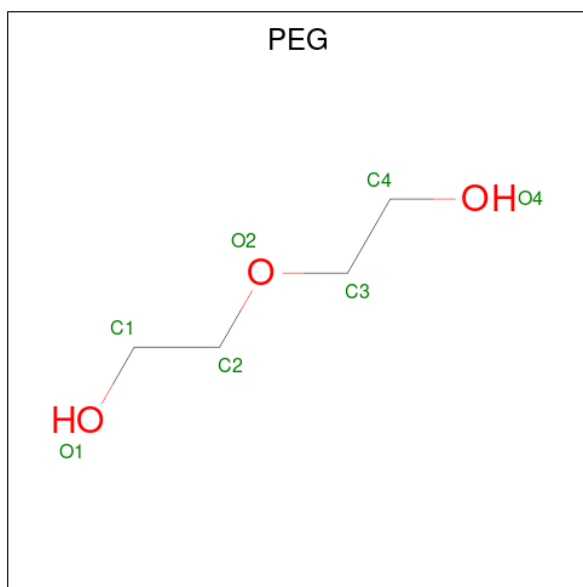
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			6	4	2		

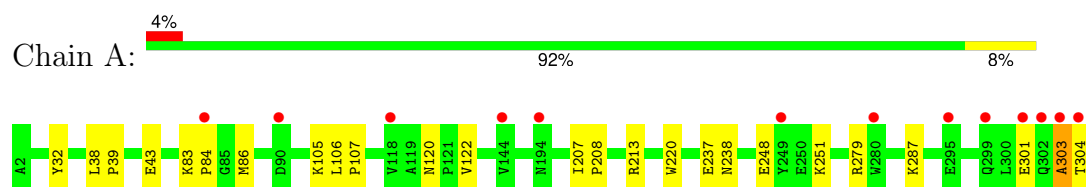
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	112	Total	O	0	0
			112	112		
9	B	114	Total	O	0	0
			114	114		

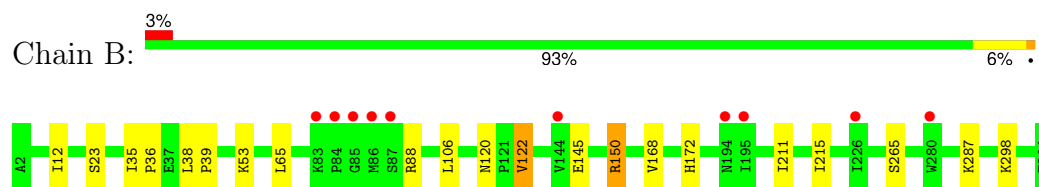
3 Residue-property plots

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: Malate dehydrogenase (NAD)



- Molecule 1: Malate dehydrogenase (NAD)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.19Å 134.19Å 81.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 31.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-1.90) 96.6 (31.05-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.226 0.202 , 0.230	Depositor DCC
R_{free} test set	3181 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5098	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PG4, PGE, MLT, PEG, EDO, GOL

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	1.01	2/2369 (0.1%)	0.89	4/3199 (0.1%)
1	B	1.00	0/2369	0.89	2/3199 (0.1%)
All	All	1.01	2/4738 (0.0%)	0.89	6/6398 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	TRP	CB-CG	-5.61	1.40	1.50
1	A	43	GLU	CD-OE2	-5.46	1.19	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ALA	N-CA-C	-5.89	95.08	111.00
1	A	279	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	150	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	213	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	53	LYS	CD-CE-NZ	5.24	123.75	111.70
1	A	105	LYS	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2326	0	2378	15	1
1	B	2326	0	2378	15	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
3	A	9	0	4	0	0
3	B	9	0	4	0	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
5	A	19	0	25	0	0
5	B	29	0	39	3	0
6	A	4	0	6	0	0
6	B	12	0	18	2	0
7	A	25	0	33	0	0
8	A	7	0	10	0	0
8	B	6	0	7	0	0
9	A	112	0	0	2	0
9	B	114	0	0	2	0
All	All	5098	0	4970	29	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 3.

All (29) 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:38:LEU:HB3	1:B:39:PRO:HD3	1.74	0.70
1:A:120:ASN:HA	1:A:122:VAL:N	2.14	0.62
1:B:120:ASN:HA	1:B:122:VAL:N	2.17	0.60
1:B:145:GLU:HB3	1:B:168:VAL:HG11	1.88	0.56
1:B:211:ILE:HG23	1:B:215:ILE:HD12	1.89	0.54
1:B:265:SER:HA	5:B:405:PGE:H2	1.91	0.51
1:A:301:GLU:O	1:A:301:GLU:HG2	2.11	0.51
1:B:23:SER:HB3	6:B:409:EDO:O2	2.11	0.49
1:A:38:LEU:N	1:A:39:PRO:CD	2.75	0.49
1:B:12:ILE:HG22	2:B:401:NAD:O1N	2.15	0.47
1:A:38:LEU:HB3	1:A:39:PRO:HD3	1.97	0.47
1:B:265:SER:HA	5:B:405:PGE:C1	2.45	0.47
1:B:88:ARG:HD2	9:B:524:HOH:O	2.15	0.46
1:A:106:LEU:N	1:A:107:PRO:CD	2.78	0.46
1:A:106:LEU:HB2	1:A:107:PRO:HD3	1.98	0.45
1:A:303:ALA:O	1:A:304:THR:OG1	2.21	0.45
1:A:301:GLU:C	1:A:303:ALA:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:HD21	1:B:150:ARG:HH22	1.66	0.44
1:A:32:TYR:CE2	2:A:401:NAD:H2A	2.53	0.43
1:A:83:LYS:HB2	1:A:86:MET:SD	2.59	0.43
1:A:237:GLU:OE2	4:B:403:GOL:C1	2.67	0.43
1:B:172:HIS:HD2	9:B:600:HOH:O	2.01	0.42
1:A:287:LYS:NZ	9:A:508:HOH:O	2.52	0.42
1:B:35:ILE:HA	1:B:36:PRO:HD3	1.88	0.42
1:A:207:ILE:HG23	1:A:208:PRO:HD3	2.02	0.42
1:B:65:LEU:HD11	1:B:106:LEU:HD21	2.01	0.42
1:B:287:LYS:NZ	6:B:407:EDO:H22	2.34	0.42
1:B:265:SER:HA	5:B:405:PGE:H12	2.02	0.41
1:A:84:PRO:HA	9:A:590:HOH:O	2.21	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)
1:A:248:GLU:OE1	1:A:251:LYS:NZ[6_554]	2.18	0.02

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	301/303 (99%)	288 (96%)	13 (4%)	0	100	100
1	B	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
All	All	602/606 (99%)	583 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	254/254 (100%)	254 (100%)	0	100	100
1	B	254/254 (100%)	252 (99%)	2 (1%)	81	82
All	All	508/508 (100%)	506 (100%)	2 (0%)	91	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	122	VAL
1	B	298	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	A	238	ASN
1	B	172	HIS
1	B	302	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

19 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$
6	EDO	B	409	-	3,3,3	0.40	0	2,2,2	0.10	0
6	EDO	A	406	-	3,3,3	0.47	0	2,2,2	0.75	0
5	PGE	B	405	-	9,9,9	0.82	0	8,8,8	0.75	0
4	GOL	A	403	-	5,5,5	0.25	0	5,5,5	0.34	0
7	PG4	A	408	-	11,11,12	0.83	0	10,10,11	0.96	1 (10%)
6	EDO	B	408	-	3,3,3	0.28	0	2,2,2	0.61	0
8	PEG	A	409	-	6,6,6	0.61	0	5,5,5	0.67	0
4	GOL	B	403	-	5,5,5	0.45	0	5,5,5	2.71	2 (40%)
5	PGE	B	404	-	9,9,9	0.78	0	8,8,8	0.77	0
5	PGE	B	406	-	8,8,9	0.93	0	7,7,8	1.39	2 (28%)
3	MLT	A	402	-	8,8,8	0.97	0	10,10,10	3.57	5 (50%)
8	PEG	B	410	-	5,5,6	0.81	0	4,4,5	0.98	0
5	PGE	A	405	-	8,8,9	0.78	0	7,7,8	1.36	1 (14%)
2	NAD	B	401	-	42,48,48	1.45	4 (9%)	50,73,73	1.62	7 (14%)
7	PG4	A	407	-	12,12,12	0.94	0	11,11,11	1.24	2 (18%)
2	NAD	A	401	-	42,48,48	1.68	7 (16%)	50,73,73	1.69	10 (20%)
6	EDO	B	407	-	3,3,3	0.33	0	2,2,2	0.48	0
3	MLT	B	402	-	8,8,8	1.28	0	10,10,10	4.15	7 (70%)
5	PGE	A	404	-	9,9,9	0.53	0	8,8,8	0.50	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
6	EDO	B	409	-	-	1/1/1/1	-
6	EDO	A	406	-	-	0/1/1/1	-
5	PGE	B	405	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	403	-	-	2/4/4/4	-
7	PG4	A	408	-	-	5/9/9/10	-
6	EDO	B	408	-	-	1/1/1/1	-
8	PEG	A	409	-	-	2/4/4/4	-
4	GOL	B	403	-	-	4/4/4/4	-
5	PGE	B	404	-	-	3/7/7/7	-
5	PGE	B	406	-	-	5/6/6/7	-
3	MLT	A	402	-	-	6/8/8/8	-
8	PEG	B	410	-	-	2/3/3/4	-
5	PGE	A	405	-	-	3/6/6/7	-
2	NAD	B	401	-	-	3/26/62/62	0/5/5/5
7	PG4	A	407	-	-	9/10/10/10	-
2	NAD	A	401	-	-	4/26/62/62	0/5/5/5
6	EDO	B	407	-	-	1/1/1/1	-
3	MLT	B	402	-	-	6/8/8/8	-
5	PGE	A	404	-	-	3/7/7/7	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	PN-O3	5.84	1.65	1.59
2	B	401	NAD	PN-O3	5.21	1.65	1.59
2	B	401	NAD	PA-O3	4.05	1.63	1.59
2	A	401	NAD	C4A-N3A	4.03	1.41	1.35
2	A	401	NAD	PA-O3	3.35	1.63	1.59
2	B	401	NAD	C2A-N3A	3.14	1.37	1.32
2	A	401	NAD	O4D-C1D	3.09	1.44	1.40
2	A	401	NAD	C2A-N3A	2.96	1.36	1.32
2	A	401	NAD	C2A-N1A	2.91	1.39	1.33
2	B	401	NAD	O4D-C1D	2.28	1.43	1.40
2	A	401	NAD	O4B-C4B	-2.08	1.40	1.45

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	MLT	O2-C1-C2	7.33	128.24	112.74
3	A	402	MLT	O1-C1-C2	-6.72	109.17	122.60
3	A	402	MLT	O2-C1-C2	6.00	125.43	112.74
2	A	401	NAD	C4B-O4B-C1B	-5.71	104.69	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	MLT	O1-C1-C2	-5.66	111.30	122.60
3	B	402	MLT	C2-C3-C4	-5.44	97.86	112.08
3	A	402	MLT	C2-C3-C4	-5.22	98.43	112.08
4	B	403	GOL	C3-C2-C1	-4.97	93.57	111.80
2	B	401	NAD	N3A-C2A-N1A	-4.76	122.22	128.67
2	B	401	NAD	C1B-N9A-C4A	-4.74	118.31	126.64
2	A	401	NAD	C1B-N9A-C4A	-4.64	118.50	126.64
2	B	401	NAD	C4B-O4B-C1B	-4.50	105.81	109.92
3	B	402	MLT	O5-C4-C3	4.35	127.54	114.00
3	B	402	MLT	O4-C4-C3	-3.87	110.97	122.84
2	A	401	NAD	O7N-C7N-C3N	3.44	123.81	119.60
2	B	401	NAD	O4B-C1B-N9A	3.24	113.05	108.75
3	A	402	MLT	O3-C2-C1	3.23	118.56	110.36
3	B	402	MLT	O3-C2-C1	3.19	118.47	110.36
4	B	403	GOL	O2-C2-C3	3.11	122.06	109.18
2	B	401	NAD	C4A-C5A-N7A	-2.85	106.33	109.34
2	B	401	NAD	O4B-C4B-C3B	2.75	110.61	105.15
5	A	405	PGE	C2-O2-C3	2.74	122.67	113.06
3	A	402	MLT	C3-C2-C1	2.51	116.70	110.53
2	A	401	NAD	O7N-C7N-N7N	-2.51	118.99	122.62
7	A	407	PG4	C3-O2-C2	2.42	123.84	113.26
5	B	406	PGE	C2-O2-C3	2.41	121.52	113.06
2	A	401	NAD	O2A-PA-O1A	2.36	123.45	112.44
3	B	402	MLT	C3-C2-C1	2.36	116.32	110.53
2	A	401	NAD	N3A-C2A-N1A	-2.30	125.55	128.67
7	A	408	PG4	O4-C7-C8	2.27	120.13	110.11
2	A	401	NAD	C4A-C5A-N7A	-2.21	107.00	109.34
2	A	401	NAD	O4B-C4B-C3B	2.10	109.32	105.15
5	B	406	PGE	O2-C3-C4	2.09	119.90	110.35
2	B	401	NAD	O2N-PN-O3	2.05	112.81	107.27
2	A	401	NAD	N6A-C6A-N1A	2.02	122.66	118.33
7	A	407	PG4	O1-C1-C2	2.02	123.72	111.82
2	A	401	NAD	C6N-N1N-C2N	-2.00	120.17	121.88

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	401	NAD	O4D-C1D-N1N-C6N
3	A	402	MLT	O1-C1-C2-O3
3	A	402	MLT	O2-C1-C2-C3
3	A	402	MLT	C1-C2-C3-C4
3	A	402	MLT	O3-C2-C3-C4
3	B	402	MLT	O2-C1-C2-C3
3	B	402	MLT	C1-C2-C3-C4
3	B	402	MLT	O3-C2-C3-C4
5	B	406	PGE	C4-C3-O2-C2
7	A	408	PG4	O3-C5-C6-O4
5	B	406	PGE	O2-C3-C4-O3
5	B	406	PGE	O3-C5-C6-O4
7	A	407	PG4	O3-C5-C6-O4
5	A	405	PGE	O2-C3-C4-O3
5	B	404	PGE	O1-C1-C2-O2
4	A	403	GOL	C1-C2-C3-O3
4	B	403	GOL	O1-C1-C2-C3
4	B	403	GOL	C1-C2-C3-O3
7	A	408	PG4	O4-C7-C8-O5
8	A	409	PEG	O1-C1-C2-O2
4	B	403	GOL	O1-C1-C2-O2
5	A	404	PGE	O3-C5-C6-O4
7	A	407	PG4	O2-C3-C4-O3
7	A	407	PG4	O4-C7-C8-O5
3	A	402	MLT	O2-C1-C2-O3
6	B	407	EDO	O1-C1-C2-O2
3	B	402	MLT	O1-C1-C2-C3
4	A	403	GOL	O2-C2-C3-O3
5	A	405	PGE	C3-C4-O3-C5
6	B	408	EDO	O1-C1-C2-O2
4	B	403	GOL	O2-C2-C3-O3
7	A	408	PG4	C4-C3-O2-C2
5	B	405	PGE	C1-C2-O2-C3
5	A	404	PGE	C3-C4-O3-C5
7	A	407	PG4	C6-C5-O3-C4
8	B	410	PEG	C1-C2-O2-C3
5	A	404	PGE	C6-C5-O3-C4
5	B	405	PGE	O1-C1-C2-O2
7	A	407	PG4	C1-C2-O2-C3
7	A	407	PG4	C8-C7-O4-C6
5	A	405	PGE	O3-C5-C6-O4
7	A	407	PG4	O1-C1-C2-O2

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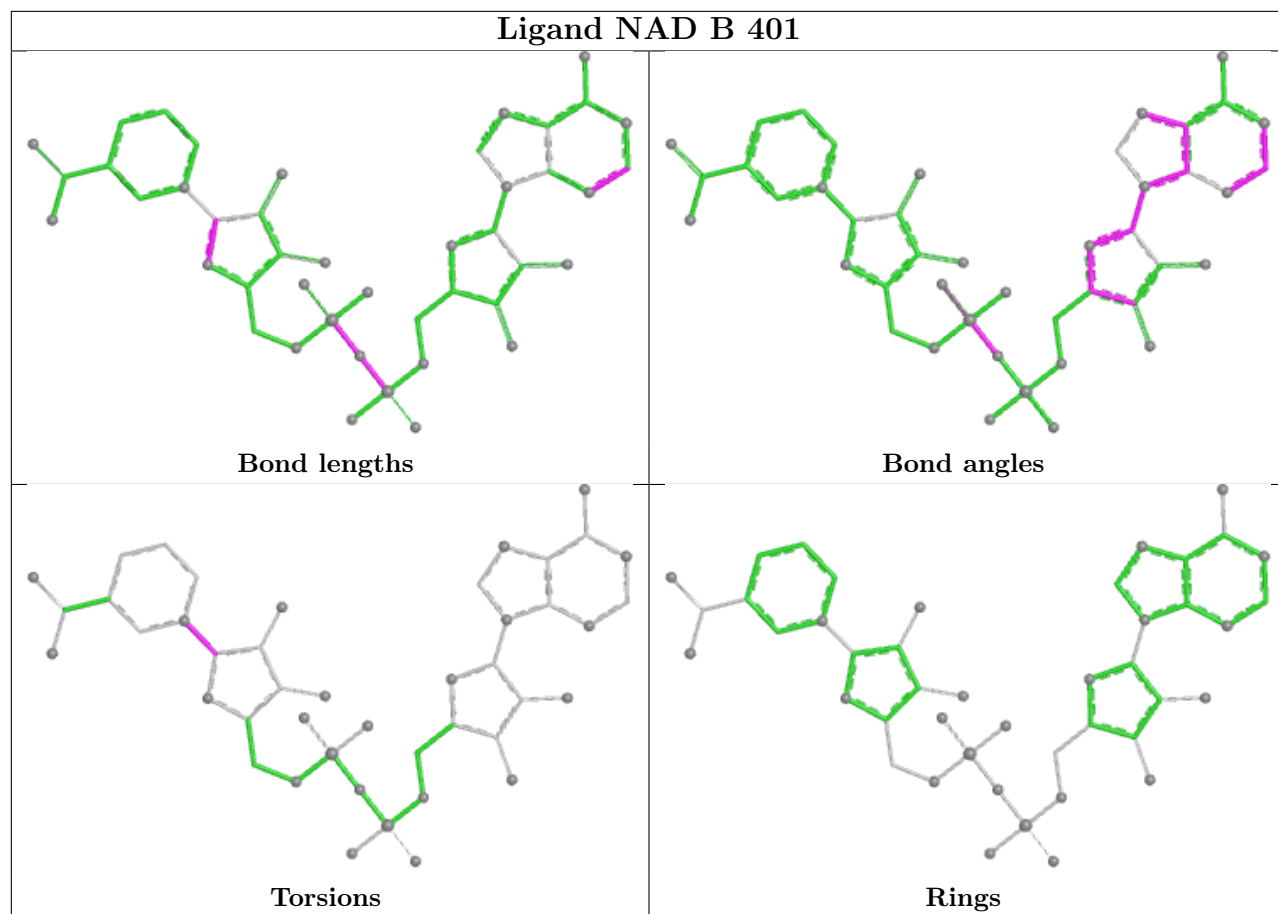
Mol	Chain	Res	Type	Atoms
5	B	404	PGE	O2-C3-C4-O3
5	B	406	PGE	C1-C2-O2-C3
3	B	402	MLT	O1-C1-C2-O3
8	B	410	PEG	C4-C3-O2-C2
6	B	409	EDO	O1-C1-C2-O2
8	A	409	PEG	C1-C2-O2-C3
7	A	408	PG4	O2-C3-C4-O3
5	B	404	PGE	C1-C2-O2-C3
5	B	406	PGE	C3-C4-O3-C5
5	B	405	PGE	C3-C4-O3-C5
5	B	405	PGE	O3-C5-C6-O4
7	A	407	PG4	C4-C3-O2-C2
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
7	A	408	PG4	C3-C4-O3-C5
3	B	402	MLT	O2-C1-C2-O3
7	A	407	PG4	C5-C6-O4-C7
3	A	402	MLT	O1-C1-C2-C3

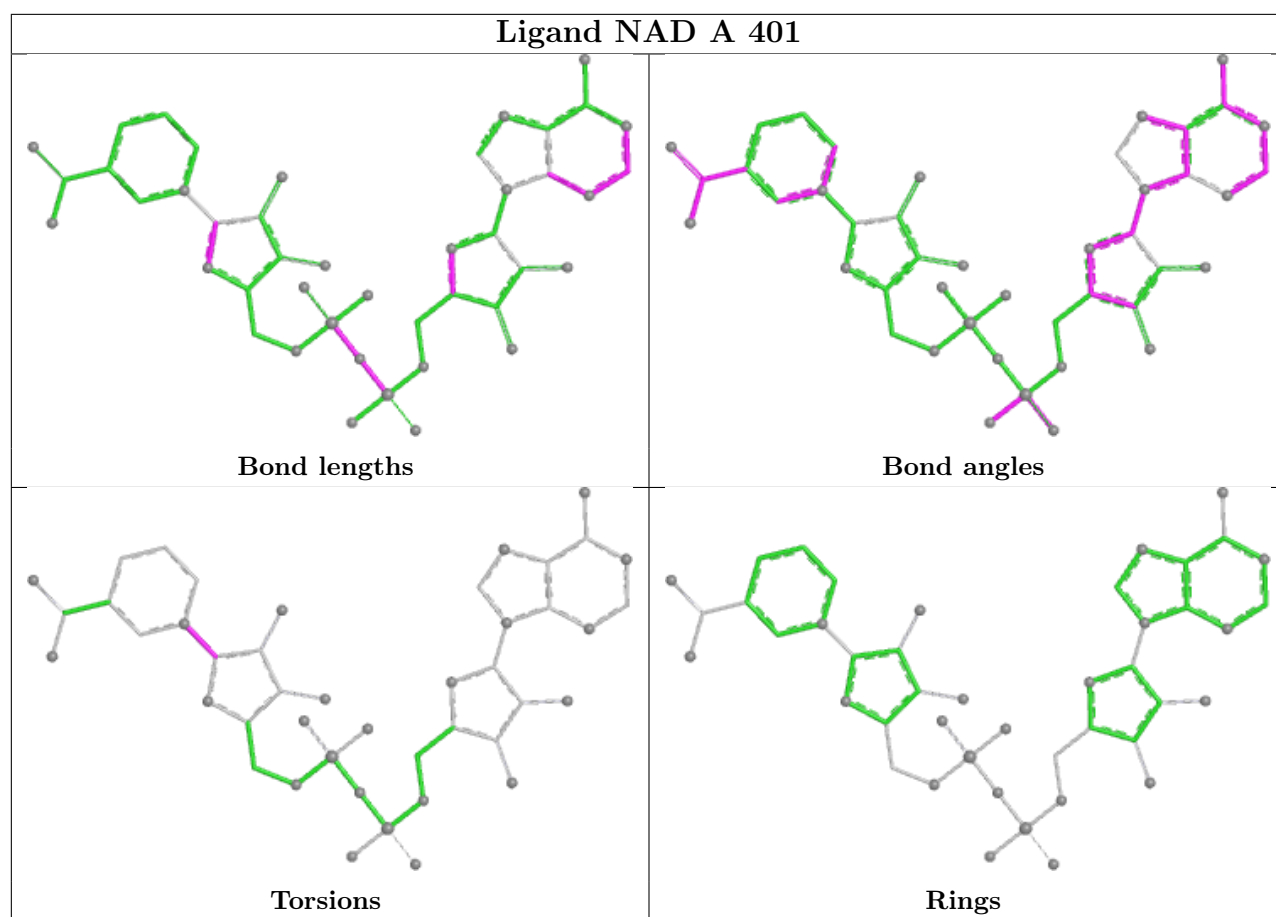
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	409	EDO	1	0
5	B	405	PGE	3	0
4	B	403	GOL	1	0
2	B	401	NAD	1	0
2	A	401	NAD	1	0
6	B	407	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 [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, 95th 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 ²)	Q<0.9
1	A	303/303 (100%)	-0.01	13 (4%) 35 38	21, 31, 60, 95	0
1	B	303/303 (100%)	-0.04	10 (3%) 46 49	21, 31, 57, 77	0
All	All	606/606 (100%)	-0.02	23 (3%) 40 43	21, 31, 59, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	PRO	6.1
1	A	303	ALA	5.5
1	A	304	THR	4.8
1	A	302	GLN	3.8
1	A	249	TYR	3.8
1	B	85	GLY	3.1
1	B	195	ILE	3.0
1	A	84	PRO	3.0
1	B	194	ASN	2.9
1	A	280	TRP	2.9
1	B	87	SER	2.8
1	A	299	GLN	2.8
1	A	194	ASN	2.7
1	B	280	TRP	2.6
1	A	295	GLU	2.5
1	A	118	VAL	2.3
1	B	83	LYS	2.3
1	B	144	VAL	2.3
1	B	86	MET	2.2
1	A	301	GLU	2.2
1	B	226	ILE	2.1
1	A	90	ASP	2.0
1	A	144	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

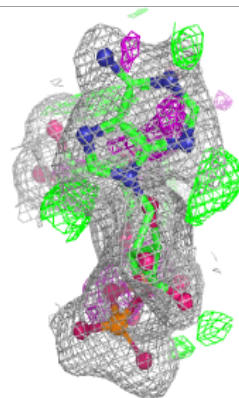
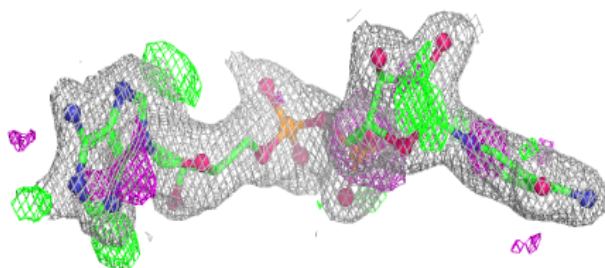
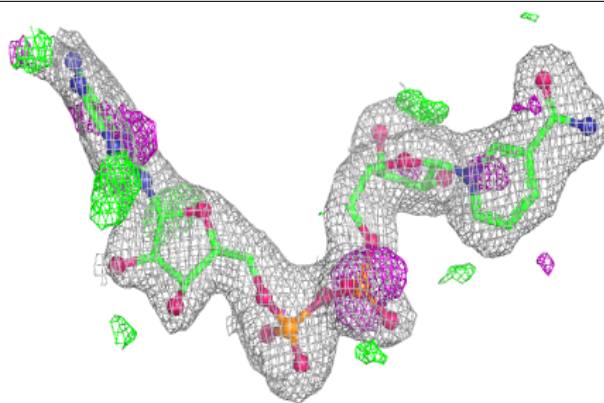
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	A	409	7/7	0.63	0.34	64,65,68,70	0
6	EDO	B	407	4/4	0.75	0.16	57,59,59,59	0
5	PGE	A	404	10/10	0.76	0.17	65,69,79,79	0
7	PG4	A	407	13/13	0.77	0.17	48,59,64,66	0
8	PEG	B	410	6/7	0.77	0.19	56,57,60,66	0
4	GOL	A	403	6/6	0.79	0.19	65,67,70,71	0
5	PGE	B	404	10/10	0.80	0.14	57,65,66,66	0
5	PGE	A	405	9/10	0.82	0.18	40,45,55,60	0
5	PGE	B	405	10/10	0.82	0.17	40,52,57,59	0
5	PGE	B	406	9/10	0.83	0.33	55,57,64,71	0
7	PG4	A	408	12/13	0.83	0.14	44,50,56,58	0
6	EDO	B	409	4/4	0.89	0.11	36,44,45,47	0
3	MLT	A	402	9/9	0.92	0.12	29,37,49,51	0
4	GOL	B	403	6/6	0.93	0.10	33,39,42,45	0
6	EDO	A	406	4/4	0.93	0.10	41,46,52,53	0
6	EDO	B	408	4/4	0.94	0.13	45,50,53,57	0
2	NAD	A	401	44/44	0.94	0.10	30,39,55,59	0
2	NAD	B	401	44/44	0.94	0.08	32,40,46,49	0
3	MLT	B	402	9/9	0.95	0.09	29,40,46,50	0

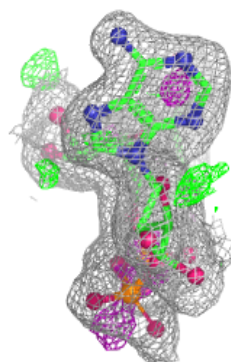
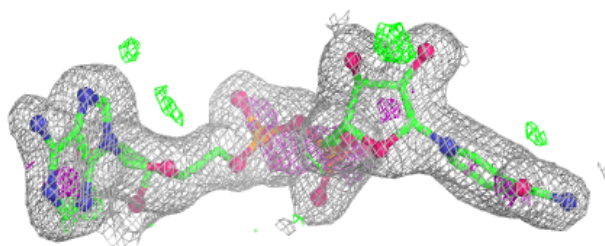
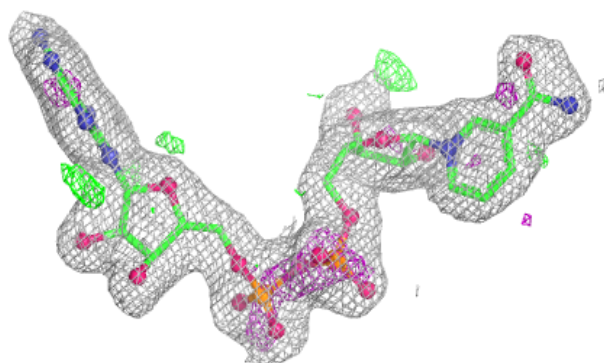
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 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 NAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.