



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:17 AM EDT

PDB ID : 5NUE
Title : Cytosolic Malate Dehydrogenase 1 (peroxide-treated)
Authors : Young, D.; Messens, J.; Huang, J.; Reichheld, J.-P.
Deposited on : 2017-04-29
Resolution : 1.35 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
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

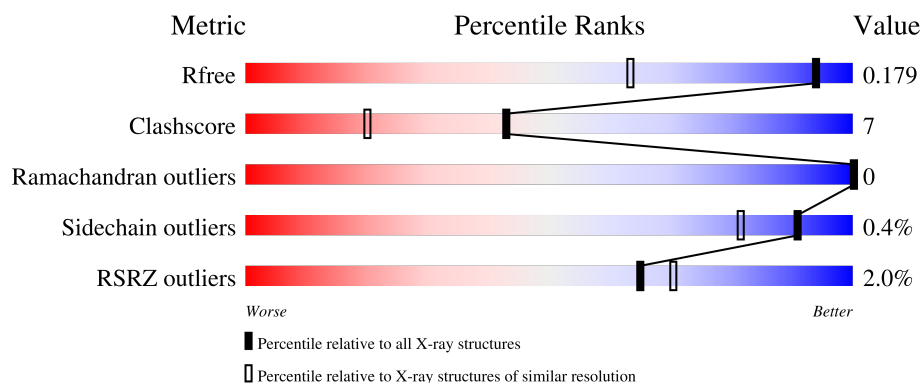
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	332	<div> <div>2%</div> <div>92%</div> <div>8%</div> </div>
2	B	332	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
3	C	332	<div> <div>3%</div> <div>91%</div> <div>8%</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
12	EDO	B	417	-	-	X	-
2	SME	B	97[A]	-	-	X	-
7	PEO	B	411	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 9265 atoms, of which 6 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 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	30	0
			2634	1678	439	499	18			

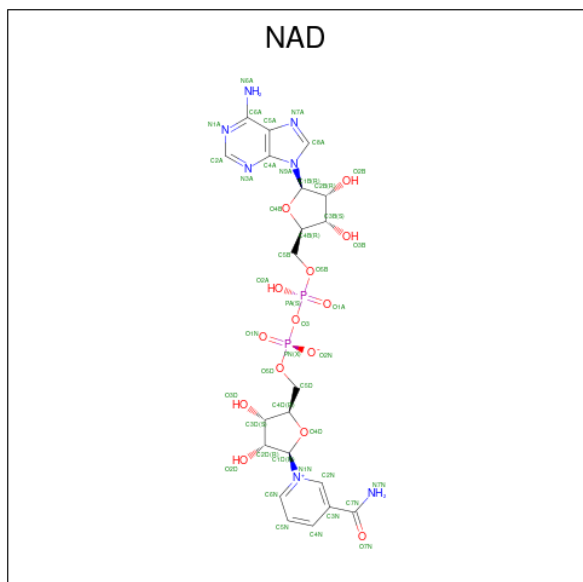
- Molecule 2 is a protein called Malate dehydrogenase 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	332	Total	C	N	O	S	0	33	0
			2670	1697	445	506	22			

- Molecule 3 is a protein called Malate dehydrogenase 1, cytoplasmic.

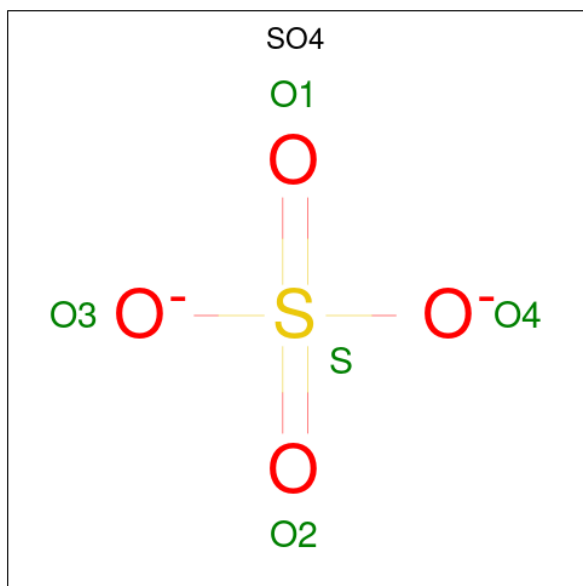
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	332	Total	C	N	O	S	0	33	0
			2673	1703	442	510	18			

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



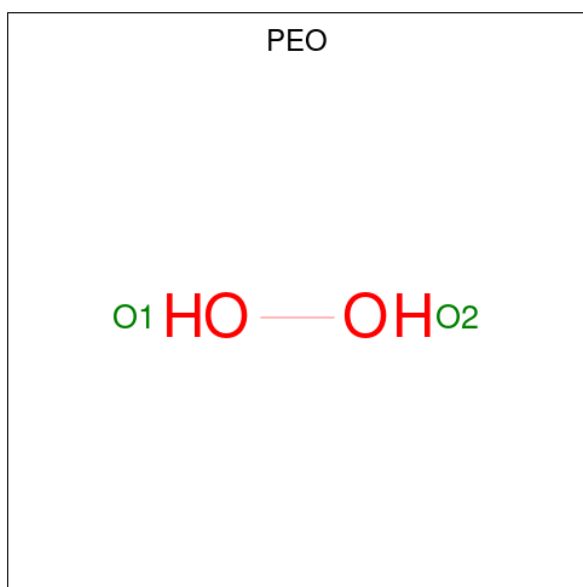
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



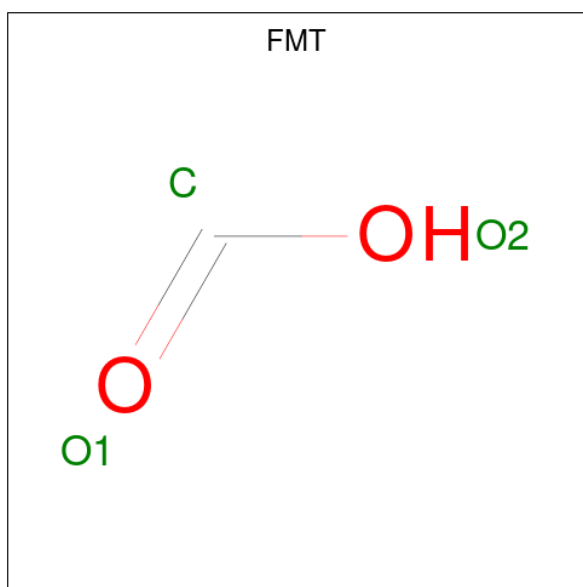
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



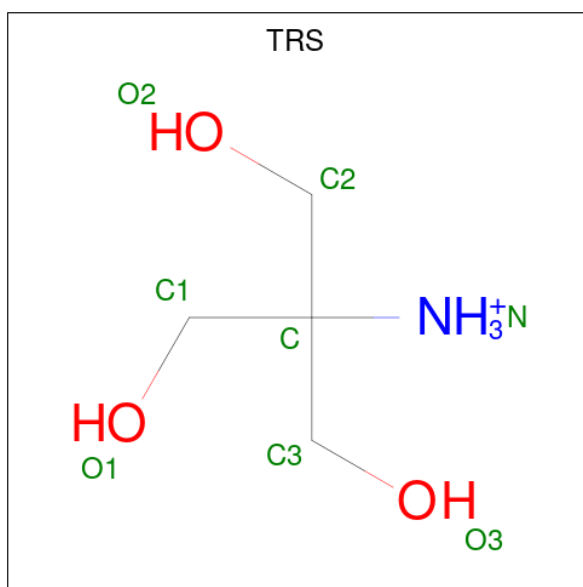
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 2 2	0	0
7	A	1	Total O 2 2	0	0
7	A	1	Total O 2 2	0	0
7	B	1	Total O 2 2	0	0
7	B	1	Total O 2 2	0	0
7	B	1	Total O 2 2	0	0
7	B	1	Total O 2 2	0	0
7	C	1	Total O 2 2	0	0
7	C	1	Total O 2 2	0	0
7	C	1	Total O 2 2	0	0
7	C	1	Total O 2 2	0	0

- Molecule 8 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



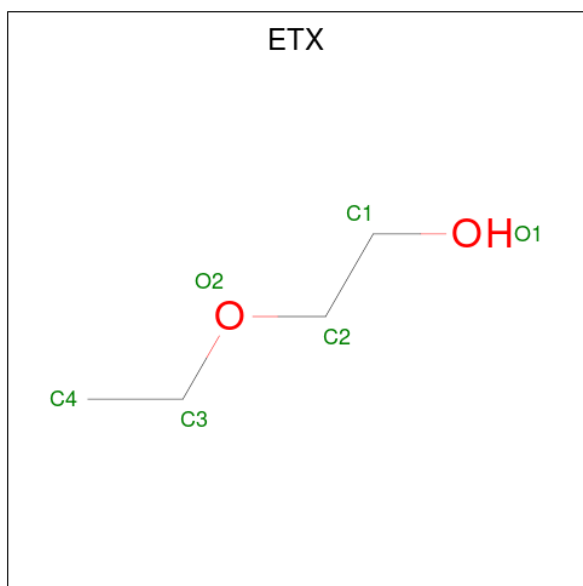
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	1	2		
8	B	1	Total	C	O	0	0
			3	1	2		
8	B	1	Total	C	O	0	0
			3	1	2		
8	C	1	Total	C	O	0	0
			3	1	2		
8	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



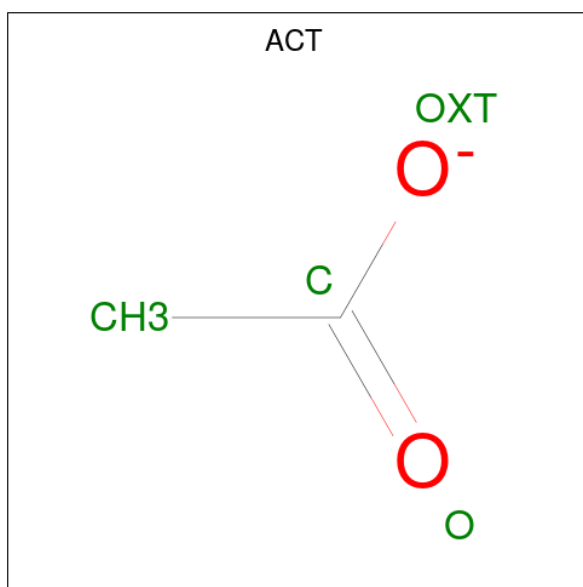
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: C₄H₁₀O₂).



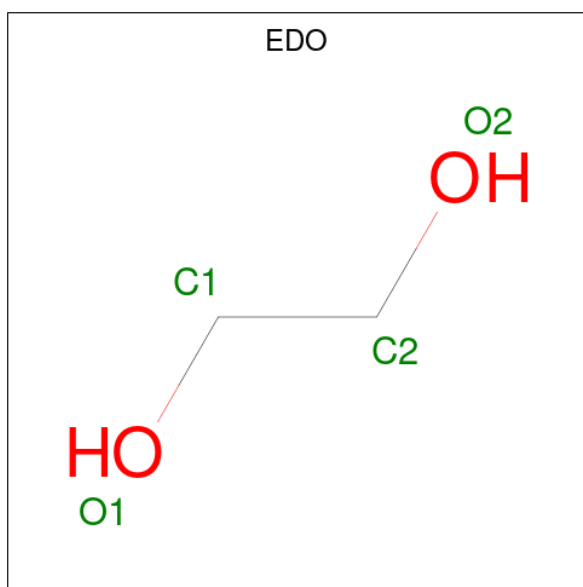
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂⁻).



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

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C H O 10 2 6 2	0	0
12	C	1	Total C O 4 2 2	0	0

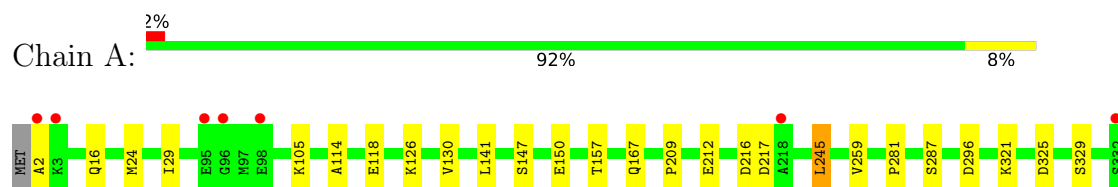
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	318	Total O 318 318	0	0
13	B	327	Total O 327 327	0	0
13	C	354	Total O 354 354	0	0

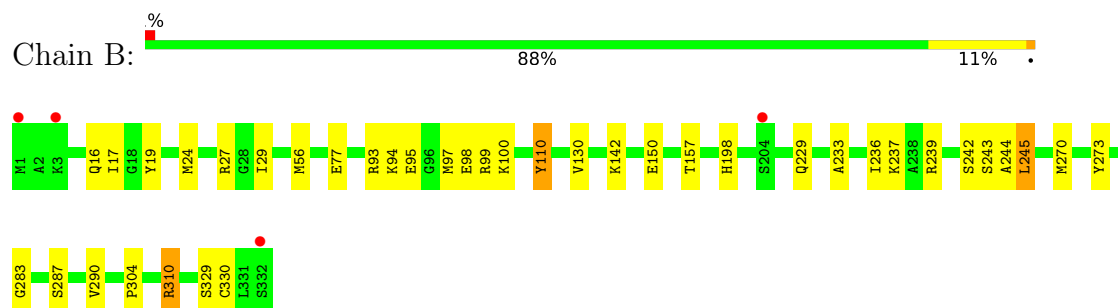
3 Residue-property plots [i](#)

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.

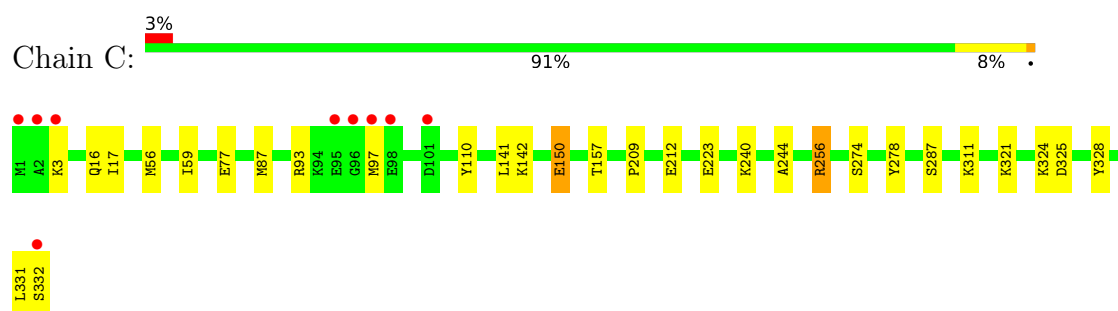
- Molecule 1: Malate dehydrogenase 1, cytoplasmic



- Molecule 2: Malate dehydrogenase 1, cytoplasmic



- Molecule 3: Malate dehydrogenase 1, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	64.60Å 118.37Å 148.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.56 – 1.35 92.56 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.56-1.35) 100.0 (92.56-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.20Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.146 , 0.180 0.146 , 0.179	Depositor DCC
R_{free} test set	17673 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9265	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEO, TRS, CSD, CSO, NAD, SME, SO4, FMT, ETX, EDO, ACT

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	0.61	0/2773	0.73	1/3754 (0.0%)
2	B	0.66	1/2762 (0.0%)	0.80	4/3735 (0.1%)
3	C	0.66	1/2787 (0.0%)	0.79	4/3771 (0.1%)
All	All	0.64	2/8322 (0.0%)	0.78	9/11260 (0.1%)

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	B	0	1
3	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	GLU	CD-OE2	-7.68	1.17	1.25
3	C	77	GLU	CD-OE2	-6.50	1.18	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	310	ARG	NE-CZ-NH2	-12.88	113.86	120.30
2	B	310	ARG	NE-CZ-NH1	11.06	125.83	120.30
3	C	325[A]	ASP	CB-CG-OD1	6.85	124.47	118.30
3	C	325[B]	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	245	LEU	CA-CB-CG	5.70	128.40	115.30
2	B	245	LEU	CA-CB-CG	5.38	127.68	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	TYR	CA-CB-CG	-5.09	103.73	113.40
3	C	256[A]	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	C	256[B]	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	110	TYR	Sidechain
3	C	110	TYR	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	2634	0	2761	27	0
2	B	2670	0	2805	49	0
3	C	2673	0	2792	35	0
4	A	44	0	26	1	0
4	B	44	0	26	2	0
4	C	44	0	26	0	0
5	A	10	0	0	0	0
5	B	15	0	0	0	0
5	C	15	0	0	1	0
6	A	12	0	16	0	0
6	B	18	0	24	2	0
6	C	6	0	8	0	0
7	A	6	0	0	0	0
7	B	8	0	0	2	0
7	C	8	0	0	0	0
8	A	3	0	1	0	0
8	B	6	0	2	0	0
8	C	6	0	2	1	0
9	A	8	0	12	5	0
10	A	6	0	10	3	0
11	B	12	0	9	0	0
12	B	8	6	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	C	4	0	6	1	0
13	A	318	0	0	8	0
13	B	327	0	0	10	0
13	C	354	0	0	17	0
All	All	9259	6	8538	114	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 7.

All (114) 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)
3:C:324:LYS:HE3	3:C:328[A]:TYR:OH	1.49	1.11
2:B:99:ARG:HH12	12:B:417:EDO:H21	1.18	1.03
2:B:229:GLN:O	12:B:417:EDO:H11	1.65	0.95
2:B:242[A]:SER:HB2	7:B:411:PEO:O2	1.68	0.92
3:C:324:LYS:HE3	3:C:328[A]:TYR:CZ	2.05	0.90
2:B:94[A]:LYS:H	2:B:97[A]:SME:HE1	1.43	0.83
10:A:411:ETX:H31	13:A:760:HOH:O	1.77	0.82
1:A:167:GLN:OE1	10:A:411:ETX:H43	1.82	0.80
1:A:150:GLU:OE2	13:A:501:HOH:O	2.00	0.80
2:B:142:LYS:HE2	2:B:150[B]:GLU:HG2	1.63	0.79
1:A:24[B]:MET:SD	1:A:29[B]:ILE:HD12	2.24	0.78
2:B:239:ARG:NH1	2:B:242[B]:SER:O	2.16	0.78
2:B:99:ARG:HH12	12:B:417:EDO:C2	1.95	0.77
1:A:217:ASP:H	9:A:410:TRS:H32	1.48	0.77
3:C:223[C]:GLU:HG3	13:C:660:HOH:O	1.85	0.77
2:B:99:ARG:NH1	12:B:417:EDO:H21	1.99	0.76
3:C:324:LYS:HE3	3:C:328[A]:TYR:CE2	2.21	0.75
3:C:331[B]:LEU:O	3:C:332:SME:OG	2.04	0.74
2:B:98:GLU:OE1	2:B:100:LYS:HE3	1.88	0.73
1:A:325[B]:ASP:OD1	13:A:502:HOH:O	2.06	0.72
2:B:94[A]:LYS:H	2:B:97[A]:SME:CE	2.02	0.72
1:A:2:ALA:O	13:A:503:HOH:O	2.11	0.68
3:C:321[B]:LYS:HE3	13:C:788:HOH:O	1.94	0.68
2:B:198[B]:HIS:CE1	2:B:304:PRO:HD2	2.29	0.67
1:A:296[A]:ASP:OD2	13:A:504:HOH:O	2.12	0.67
6:B:406:GOL:H32	13:B:541:HOH:O	1.95	0.67
2:B:239:ARG:NH1	2:B:242[C]:SER:O	2.27	0.67
1:A:24[B]:MET:SD	1:A:29[B]:ILE:CD1	2.85	0.65
2:B:310:ARG:O	2:B:310:ARG:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASP:H	9:A:410:TRS:C3	2.12	0.62
2:B:24[A]:MET:SD	2:B:29[A]:ILE:HD12	2.40	0.62
2:B:95:GLU:OE2	2:B:237:LYS:HD2	1.99	0.62
3:C:274[B]:SER:OG	13:C:502:HOH:O	2.14	0.62
3:C:324:LYS:CE	3:C:328[A]:TYR:CE2	2.84	0.60
10:A:411:ETX:C3	13:A:760:HOH:O	2.43	0.59
3:C:142[B]:LYS:HE2	3:C:150[B]:GLU:HG2	1.85	0.59
2:B:24[A]:MET:SD	2:B:29[A]:ILE:CD1	2.91	0.58
2:B:236[A]:ILE:HG13	2:B:242[A]:SER:HA	1.86	0.58
1:A:16[B]:GLN:CG	13:A:655:HOH:O	2.51	0.58
3:C:331[B]:LEU:O	3:C:332:SER:CB	2.53	0.57
1:A:281:PRO:HG2	1:A:321[B]:LYS:HE3	1.87	0.57
1:A:217:ASP:N	9:A:410:TRS:H32	2.17	0.57
3:C:278:TYR:HA	12:C:412:EDO:H12	1.85	0.57
5:C:403:SO4:O2	13:C:501:HOH:O	2.14	0.57
2:B:236[A]:ILE:CG1	2:B:242[A]:SER:HA	2.34	0.57
3:C:240:LYS:HE2	13:C:542:HOH:O	2.04	0.56
2:B:24[B]:MET:CE	13:B:719:HOH:O	2.52	0.56
2:B:16[B]:GLN:OE1	13:B:501:HOH:O	2.18	0.56
3:C:321[B]:LYS:CE	13:C:788:HOH:O	2.52	0.56
2:B:93:ARG:HA	2:B:97[A]:SME:HE1	1.88	0.56
1:A:16[B]:GLN:HG3	13:A:655:HOH:O	2.05	0.55
3:C:324:LYS:HG3	3:C:328[A]:TYR:CZ	2.42	0.54
3:C:3:LYS:HE2	13:C:637:HOH:O	2.06	0.54
3:C:321[B]:LYS:HE3	13:C:673:HOH:O	2.07	0.54
2:B:233:ALA:O	2:B:236[B]:ILE:HG22	2.08	0.54
2:B:236[A]:ILE:HD11	2:B:242[A]:SER:HB3	1.89	0.54
3:C:93:ARG:NH1	3:C:97:MET:O	2.42	0.53
3:C:209[A]:PRO:HG2	3:C:212:GLU:HB2	1.90	0.53
3:C:321[B]:LYS:HG3	13:C:673:HOH:O	2.08	0.53
3:C:16[B]:GLN:HG3	13:C:625:HOH:O	2.08	0.52
3:C:59[A]:ILE:HD11	13:C:787:HOH:O	2.09	0.52
1:A:118:GLU:HG3	1:A:147:SER:OG	2.10	0.52
2:B:142:LYS:HE2	2:B:150[B]:GLU:CG	2.36	0.51
3:C:324:LYS:CE	3:C:328[A]:TYR:OH	2.41	0.51
3:C:142[B]:LYS:HD2	13:C:659:HOH:O	2.09	0.51
1:A:209[A]:PRO:HG2	1:A:212:GLU:HB2	1.92	0.51
3:C:142[B]:LYS:CD	13:C:659:HOH:O	2.58	0.51
2:B:243[A]:SER:N	7:B:411:PEO:O2	2.36	0.51
2:B:94[A]:LYS:HD2	13:B:742:HOH:O	2.10	0.50
2:B:24[B]:MET:HE2	13:B:719:HOH:O	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:GLN:C	12:B:417:EDO:H11	2.32	0.50
1:A:157:THR:HG21	1:A:287:SER:HB2	1.94	0.50
2:B:273:TYR:CZ	2:B:283:GLY:HA2	2.46	0.50
2:B:93:ARG:CA	2:B:97[A]:SME:HE1	2.43	0.49
1:A:29[B]:ILE:HD13	2:B:27:ARG:HG2	1.94	0.49
2:B:130:VAL:O	4:B:401:NAD:H2N	2.13	0.49
3:C:16[B]:GLN:CG	13:C:625:HOH:O	2.59	0.49
2:B:236[A]:ILE:HG12	2:B:242[A]:SER:CA	2.42	0.49
2:B:19:TYR:HB2	13:B:589:HOH:O	2.11	0.48
6:B:406:GOL:H2	13:B:749:HOH:O	2.12	0.48
3:C:157:THR:HG21	3:C:287:SER:HB2	1.96	0.48
2:B:93:ARG:HA	2:B:97[A]:SME:CE	2.44	0.47
2:B:242[C]:SER:HB2	4:B:401:NAD:O1N	2.13	0.47
2:B:16[A]:GLN:HG3	13:B:501:HOH:O	2.14	0.47
3:C:324:LYS:CE	3:C:328[A]:TYR:HE2	2.27	0.46
1:A:329:SER:HB3	3:C:209[B]:PRO:HG3	1.96	0.46
1:A:209[A]:PRO:HG2	1:A:212:GLU:CB	2.46	0.46
1:A:329:SER:CB	3:C:209[B]:PRO:HG3	2.46	0.46
3:C:256[A]:ARG:NH2	13:C:509:HOH:O	2.42	0.46
2:B:310:ARG:HD3	2:B:310:ARG:C	2.38	0.44
1:A:216:ASP:CA	9:A:410:TRS:H32	2.48	0.44
2:B:236[A]:ILE:CD1	2:B:242[A]:SER:HB3	2.47	0.44
3:C:87[B]:MET:SD	3:C:141:LEU:HD11	2.58	0.44
2:B:242[A]:SER:CB	13:B:503:HOH:O	2.66	0.43
1:A:216:ASP:HA	9:A:410:TRS:H32	2.01	0.43
2:B:93:ARG:HB2	2:B:97[A]:SME:HB3	2.00	0.43
1:A:114:ALA:HB2	1:A:141[A]:LEU:HD12	2.00	0.43
2:B:24[B]:MET:HE3	13:B:719:HOH:O	2.17	0.43
2:B:27:ARG:HA	2:B:27:ARG:HD3	1.85	0.43
1:A:105:LYS:HB3	1:A:105:LYS:HE3	1.81	0.43
2:B:236[A]:ILE:HG12	2:B:242[A]:SER:HA	2.01	0.42
2:B:329[A]:SER:OG	12:B:418:EDO:H12	2.19	0.42
3:C:209[A]:PRO:HG2	3:C:212:GLU:CB	2.49	0.42
1:A:126[B]:LYS:HD2	1:A:259:VAL:HG22	2.02	0.41
1:A:130:VAL:O	4:A:401:NAD:H2N	2.21	0.41
3:C:17:ILE:HG12	3:C:244:ALA:HA	2.03	0.41
3:C:311[B]:LYS:HE3	13:C:810:HOH:O	2.21	0.41
2:B:270:MET:SD	2:B:290:VAL:HG21	2.61	0.41
8:C:411:FMT:H	13:C:678:HOH:O	2.21	0.41
2:B:17:ILE:HG12	2:B:244:ALA:HA	2.03	0.40
2:B:157:THR:HG21	2:B:287:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/332 (109%)	352 (98%)	9 (2%)	0	100	100
2	B	359/332 (108%)	353 (98%)	6 (2%)	0	100	100
3	C	362/332 (109%)	355 (98%)	7 (2%)	0	100	100
All	All	1082/996 (109%)	1060 (98%)	22 (2%)	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	302/273 (111%)	301 (100%)	1 (0%)	92	83
2	B	302/270 (112%)	301 (100%)	1 (0%)	92	83
3	C	304/271 (112%)	302 (99%)	2 (1%)	84	64
All	All	908/814 (112%)	904 (100%)	4 (0%)	91	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LEU
2	B	245	LEU

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Mol	Chain	Res	Type
3	C	150[A]	GLU
3	C	150[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	CSD	B	330[B]	-	3,7,8	0.89	0	1,8,10	0.57	0
2	SME	B	97[B]	-	7,8,9	1.18	0	4,9,11	0.57	0
2	SME	B	56	2	7,8,9	2.23	2 (28%)	4,9,11	2.73	1 (25%)
3	CSO	C	330	3	3,6,7	0.57	0	0,6,8	-	-
2	CSD	B	330[A]	-	3,5,8	0.80	0	1,5,10	3.21	1 (100%)
2	SME	B	97[A]	-	7,8,9	1.12	0	4,9,11	1.25	0
3	SME	C	56[B]	-	7,8,9	1.08	0	4,9,11	2.95	2 (50%)
3	SME	C	56[A]	-	7,8,9	0.94	0	4,9,11	1.27	1 (25%)

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	CSD	B	330[B]	-	-	1/2/6/8	-
2	SME	B	97[B]	-	-	4/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SME	B	56	2	-	1/6/7/9	-
3	CSO	C	330	3	-	0/1/5/7	-
2	CSD	B	330[A]	-	-	1/2/4/8	-
2	SME	B	97[A]	-	-	3/6/7/9	-
3	SME	C	56[B]	-	-	0/6/7/9	-
3	SME	C	56[A]	-	-	2/6/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	56	SME	CE-S	-4.96	1.54	1.77
2	B	56	SME	CB-CA	2.34	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	SME	OE-S-CG	5.45	121.06	106.03
3	C	56[B]	SME	OE-S-CG	4.44	118.27	106.03
3	C	56[B]	SME	CE-S-CG	3.72	106.19	97.71
2	B	330[A]	CSD	OD1-SG-CB	-3.21	99.43	105.54
3	C	56[A]	SME	OE-S-CE	-2.15	101.90	106.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	97[B]	SME	C-CA-CB-CG
2	B	97[B]	SME	CB-CG-S-OE
2	B	330[A]	CSD	CA-CB-SG-OD1
2	B	330[B]	CSD	CA-CB-SG-OD1
3	C	56[A]	SME	CB-CG-S-OE
3	C	56[A]	SME	CB-CG-S-CE
2	B	97[B]	SME	CB-CG-S-CE
2	B	97[A]	SME	CB-CG-S-OE
2	B	97[A]	SME	CB-CG-S-CE
2	B	56	SME	CB-CG-S-OE
2	B	97[B]	SME	N-CA-CB-CG
2	B	97[A]	SME	CA-CB-CG-S

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	97[A]	SME	7	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

41 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PEO	C	408	-	1,1,1	0.23	0	-		
12	EDO	B	418	-	3,3,3	0.51	0	2,2,2	0.48	0
5	SO4	C	403	-	4,4,4	0.24	0	6,6,6	0.67	0
12	EDO	C	412	-	3,3,3	0.47	0	2,2,2	0.47	0
7	PEO	B	408	-	1,1,1	0.18	0	-		
6	GOL	B	406	-	5,5,5	0.82	0	5,5,5	1.07	0
8	FMT	C	410	-	2,2,2	0.59	0	1,1,1	0.81	0
11	ACT	B	412	-	3,3,3	0.76	0	3,3,3	1.18	0
8	FMT	B	415	-	2,2,2	0.65	0	1,1,1	0.57	0
6	GOL	B	407	-	5,5,5	0.93	0	5,5,5	1.22	1 (20%)
5	SO4	A	402	-	4,4,4	0.16	0	6,6,6	0.47	0
5	SO4	B	403	-	4,4,4	0.34	0	6,6,6	1.44	1 (16%)
7	PEO	C	407	-	1,1,1	0.04	0	-		
8	FMT	A	409	-	2,2,2	0.62	0	1,1,1	0.81	0
6	GOL	B	405	-	5,5,5	0.94	0	5,5,5	0.94	0
7	PEO	C	409	-	1,1,1	0.15	0	-		
5	SO4	C	402	-	4,4,4	0.20	0	6,6,6	0.87	0
10	ETX	A	411	-	5,5,5	0.51	0	4,4,4	0.89	0
4	NAD	A	401	-	42,48,48	3.18	10 (23%)	50,73,73	2.10	9 (18%)
11	ACT	B	413	-	3,3,3	0.90	0	3,3,3	1.10	0
12	EDO	B	417	-	3,3,3	0.58	0	2,2,2	0.48	0
7	PEO	C	406	-	1,1,1	0.03	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	ACT	B	414	-	3,3,3	0.99	0	3,3,3	0.81	0
7	PEO	B	411	-	1,1,1	0.10	0	-		
7	PEO	A	406	-	1,1,1	0.01	0	-		
6	GOL	C	405	-	5,5,5	1.31	1 (20%)	5,5,5	1.14	0
8	FMT	B	416	-	2,2,2	0.51	0	1,1,1	0.67	0
6	GOL	A	404	-	5,5,5	1.58	1 (20%)	5,5,5	1.11	1 (20%)
8	FMT	C	411	-	2,2,2	0.60	0	1,1,1	0.60	0
5	SO4	B	402	-	4,4,4	0.12	0	6,6,6	0.59	0
4	NAD	B	401	-	42,48,48	2.90	9 (21%)	50,73,73	2.26	10 (20%)
7	PEO	B	409	-	1,1,1	0.13	0	-		
4	NAD	C	401	-	42,48,48	3.07	13 (30%)	50,73,73	2.24	15 (30%)
7	PEO	A	408	-	1,1,1	0.08	0	-		
6	GOL	A	405	-	5,5,5	0.99	0	5,5,5	1.17	0
5	SO4	C	404	-	4,4,4	0.34	0	6,6,6	0.36	0
5	SO4	A	403	-	4,4,4	0.18	0	6,6,6	0.29	0
5	SO4	B	404	-	4,4,4	0.28	0	6,6,6	0.29	0
7	PEO	B	410	-	1,1,1	0.31	0	-		
9	TRS	A	410	-	7,7,7	0.64	0	9,9,9	1.01	0
7	PEO	A	407	-	1,1,1	0.55	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
12	EDO	B	418	-	-	1/1/1/1	-
6	GOL	B	407	-	-	3/4/4/4	-
6	GOL	C	405	-	-	2/4/4/4	-
6	GOL	A	404	-	-	0/4/4/4	-
12	EDO	C	412	-	-	0/1/1/1	-
6	GOL	B	405	-	-	0/4/4/4	-
10	ETX	A	411	-	-	1/3/3/3	-
6	GOL	B	406	-	-	2/4/4/4	-
4	NAD	A	401	-	-	5/26/62/62	0/5/5/5
12	EDO	B	417	-	-	1/1/1/1	-
9	TRS	A	410	-	-	3/9/9/9	-
4	NAD	B	401	-	-	5/26/62/62	0/5/5/5
4	NAD	C	401	-	-	5/26/62/62	0/5/5/5
6	GOL	A	405	-	-	4/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	NAD	C2D-C1D	-11.56	1.36	1.53
4	A	401	NAD	O4D-C1D	11.00	1.56	1.41
4	A	401	NAD	C2D-C1D	-10.82	1.37	1.53
4	C	401	NAD	O4D-C1D	10.30	1.55	1.41
4	B	401	NAD	C2D-C1D	-10.03	1.38	1.53
4	B	401	NAD	O4D-C1D	9.60	1.54	1.41
4	A	401	NAD	C3B-C4B	-6.74	1.35	1.53
4	A	401	NAD	O4B-C4B	5.80	1.58	1.45
4	C	401	NAD	O4B-C4B	5.60	1.57	1.45
4	B	401	NAD	O4B-C4B	5.34	1.56	1.45
4	B	401	NAD	C3B-C4B	-5.11	1.39	1.53
4	C	401	NAD	C3B-C4B	-4.96	1.40	1.53
4	A	401	NAD	O4B-C1B	-4.74	1.34	1.41
4	C	401	NAD	O4B-C1B	-4.37	1.35	1.41
4	B	401	NAD	C7N-N7N	4.28	1.41	1.33
4	B	401	NAD	O4B-C1B	-4.25	1.35	1.41
4	B	401	NAD	C6A-N6A	3.36	1.46	1.34
4	C	401	NAD	C7N-N7N	3.35	1.39	1.33
4	A	401	NAD	O4D-C4D	-3.29	1.37	1.45
4	C	401	NAD	O4D-C4D	-3.27	1.37	1.45
4	A	401	NAD	C6A-N6A	3.22	1.45	1.34
4	B	401	NAD	O4D-C4D	-2.95	1.38	1.45
4	A	401	NAD	O2D-C2D	2.92	1.49	1.43
4	B	401	NAD	O2D-C2D	2.78	1.49	1.43
4	C	401	NAD	O2D-C2D	2.73	1.49	1.43
4	C	401	NAD	C6A-N6A	2.70	1.43	1.34
4	C	401	NAD	C2A-N1A	2.69	1.38	1.33
4	C	401	NAD	C2A-N3A	2.62	1.36	1.32
4	A	401	NAD	C2N-N1N	2.55	1.38	1.35
4	A	401	NAD	O3B-C3B	2.54	1.49	1.43
4	C	401	NAD	O3B-C3B	2.50	1.48	1.43
6	A	404	GOL	O2-C2	2.24	1.50	1.43
6	C	405	GOL	O2-C2	-2.11	1.37	1.43
4	C	401	NAD	C5D-C4D	2.08	1.58	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	NAD	C1B-N9A-C4A	-8.18	112.26	126.64
4	C	401	NAD	C1B-N9A-C4A	-8.10	112.41	126.64
4	B	401	NAD	C1B-N9A-C4A	-7.05	114.25	126.64
4	B	401	NAD	N3A-C2A-N1A	-6.17	119.03	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	NAD	O7N-C7N-C3N	5.67	126.42	119.63
4	C	401	NAD	O7N-C7N-C3N	5.53	126.25	119.63
4	A	401	NAD	O7N-C7N-C3N	5.35	126.03	119.63
4	B	401	NAD	O4D-C1D-C2D	-5.05	99.55	106.93
4	C	401	NAD	N3A-C2A-N1A	-4.82	121.14	128.68
4	B	401	NAD	C3N-C7N-N7N	-4.74	112.07	117.75
4	A	401	NAD	O4D-C1D-C2D	-4.68	100.09	106.93
4	C	401	NAD	O4D-C1D-C2D	-4.29	100.66	106.93
4	B	401	NAD	C5A-C6A-N6A	4.19	126.72	120.35
4	C	401	NAD	O4B-C1B-C2B	-4.09	100.95	106.93
4	C	401	NAD	C3N-C7N-N7N	-3.78	113.21	117.75
4	A	401	NAD	C5A-C6A-N6A	3.54	125.73	120.35
4	B	401	NAD	O4B-C1B-C2B	-3.43	101.92	106.93
4	A	401	NAD	N3A-C2A-N1A	-3.20	123.67	128.68
4	A	401	NAD	C3N-C7N-N7N	-3.14	113.98	117.75
4	A	401	NAD	O4B-C1B-C2B	-3.07	102.44	106.93
4	C	401	NAD	C3D-C2D-C1D	2.95	105.42	100.98
4	C	401	NAD	C2D-C3D-C4D	-2.89	97.03	102.64
4	A	401	NAD	C5N-C4N-C3N	2.86	123.73	120.34
4	B	401	NAD	C2D-C3D-C4D	-2.77	97.25	102.64
4	C	401	NAD	C6N-N1N-C2N	-2.64	119.56	121.97
4	C	401	NAD	C2B-C3B-C4B	2.57	107.63	102.64
4	C	401	NAD	C5A-C6A-N6A	2.56	124.23	120.35
4	B	401	NAD	C6N-N1N-C2N	-2.50	119.70	121.97
4	C	401	NAD	O4D-C4D-C3D	2.49	110.04	105.11
5	B	403	SO4	O4-S-O1	-2.43	96.62	109.31
4	A	401	NAD	C3D-C2D-C1D	2.38	104.57	100.98
4	C	401	NAD	O5B-C5B-C4B	-2.28	101.14	108.99
4	B	401	NAD	O4B-C4B-C5B	-2.25	101.96	109.37
4	C	401	NAD	PN-O3-PA	-2.18	125.35	132.83
6	B	407	GOL	C3-C2-C1	-2.11	103.49	111.70
6	A	404	GOL	C3-C2-C1	-2.10	103.55	111.70
4	C	401	NAD	O4B-C4B-C5B	-2.08	102.52	109.37

There are no chirality outliers.

All (32) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
4	B	401	NAD	O4D-C1D-N1N-C2N
4	B	401	NAD	O4D-C1D-N1N-C6N
4	B	401	NAD	C2D-C1D-N1N-C2N
4	B	401	NAD	C2D-C1D-N1N-C6N
4	C	401	NAD	O4D-C1D-N1N-C2N
4	C	401	NAD	O4D-C1D-N1N-C6N
4	C	401	NAD	C2D-C1D-N1N-C2N
4	C	401	NAD	C2D-C1D-N1N-C6N
6	A	405	GOL	O1-C1-C2-O2
6	A	405	GOL	O1-C1-C2-C3
6	A	405	GOL	C1-C2-C3-O3
6	B	406	GOL	C1-C2-C3-O3
6	C	405	GOL	C1-C2-C3-O3
6	B	406	GOL	O2-C2-C3-O3
6	C	405	GOL	O2-C2-C3-O3
12	B	417	EDO	O1-C1-C2-O2
12	B	418	EDO	O1-C1-C2-O2
9	A	410	TRS	C1-C-C3-O3
6	B	407	GOL	O1-C1-C2-O2
6	B	407	GOL	O2-C2-C3-O3
9	A	410	TRS	N-C-C3-O3
9	A	410	TRS	C2-C-C3-O3
6	A	405	GOL	O2-C2-C3-O3
6	B	407	GOL	O1-C1-C2-C3
10	A	411	ETX	C4-C3-O2-C2
4	A	401	NAD	O4B-C4B-C5B-O5B
4	B	401	NAD	O4B-C4B-C5B-O5B
4	C	401	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

11 monomers are involved in 24 short contacts:

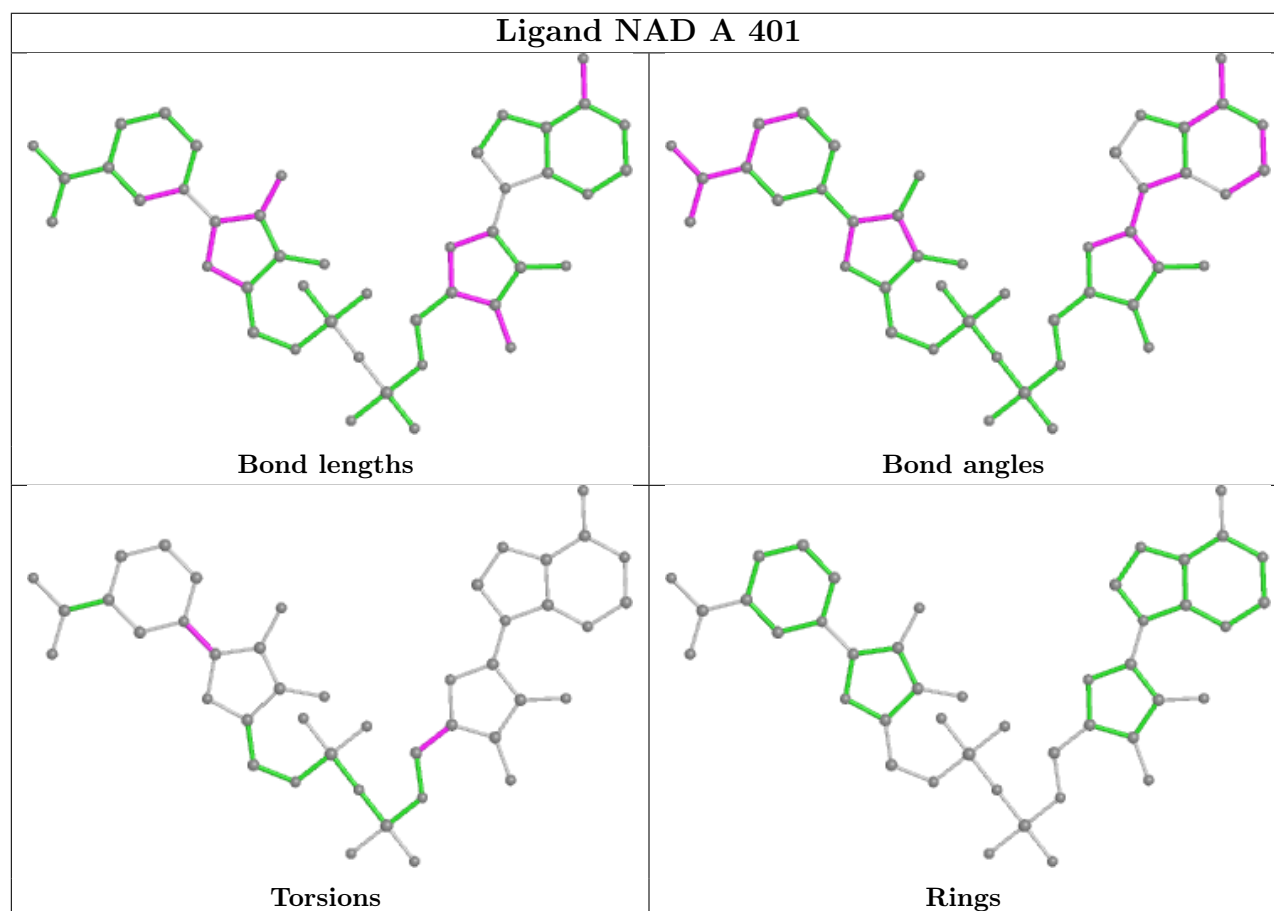
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	418	EDO	1	0
5	C	403	SO4	1	0
12	C	412	EDO	1	0
6	B	406	GOL	2	0
10	A	411	ETX	3	0
4	A	401	NAD	1	0
12	B	417	EDO	5	0
7	B	411	PEO	2	0
8	C	411	FMT	1	0

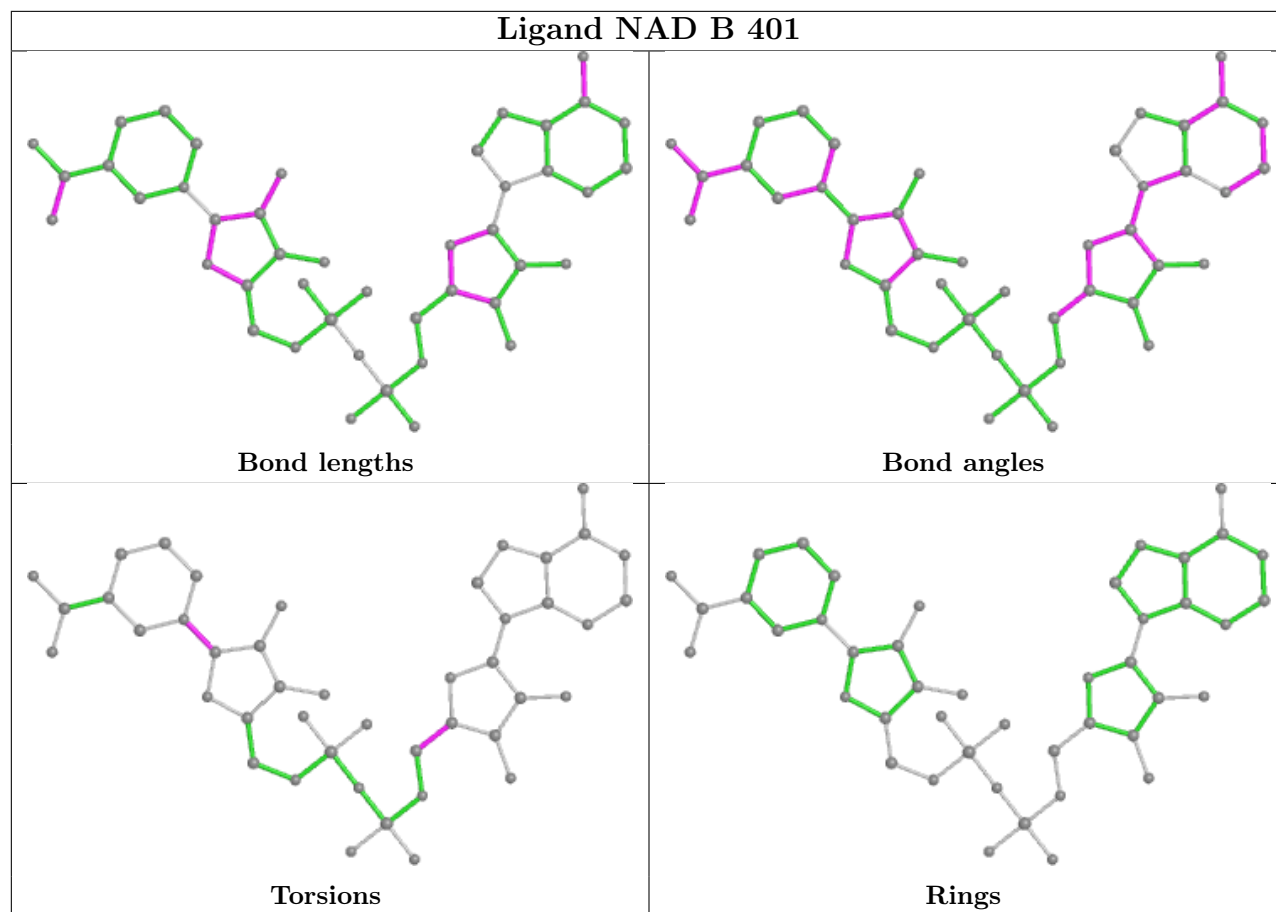
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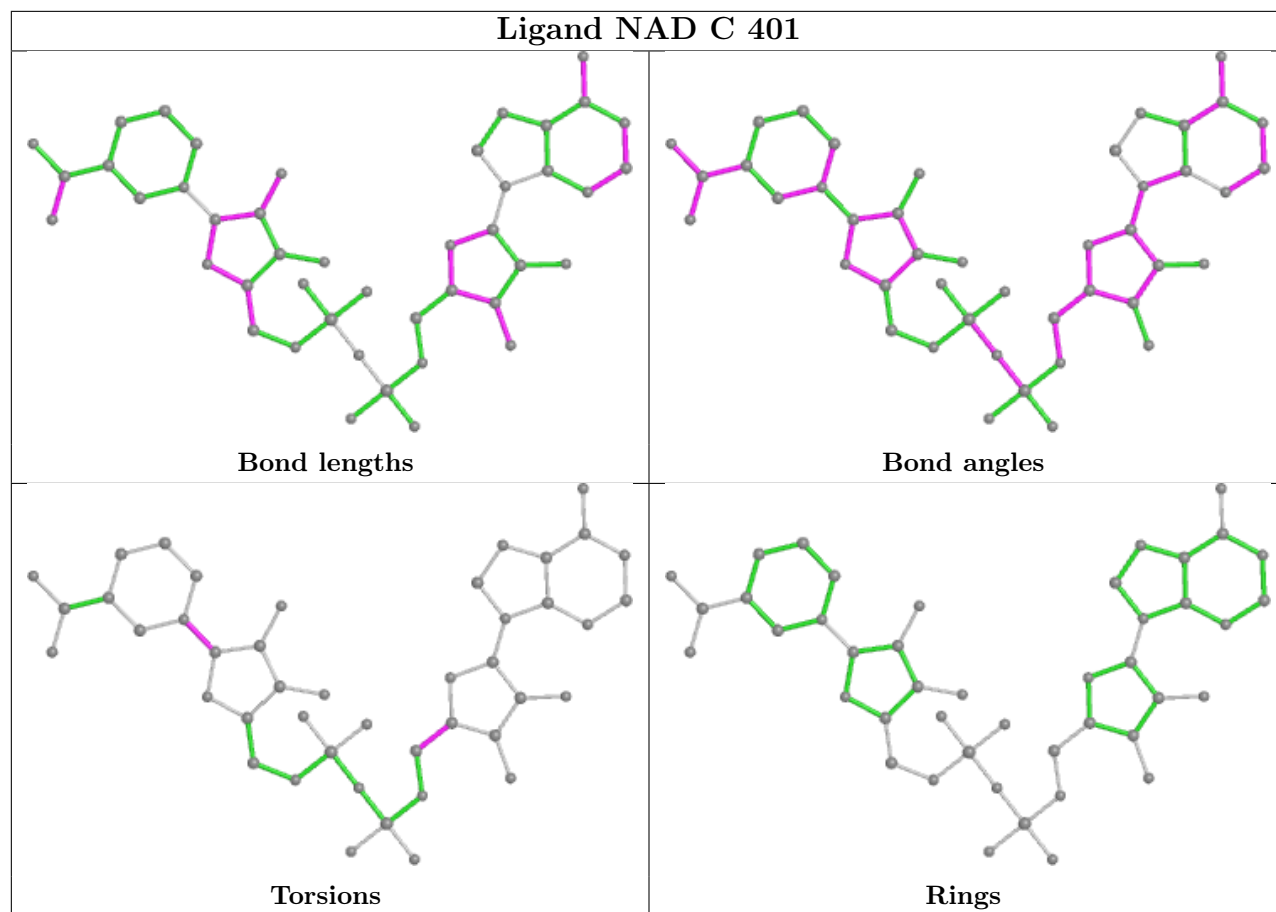
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	NAD	2	0
9	A	410	TRS	5	0

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	331/332 (99%)	-0.19	7 (2%) 63 69	11, 18, 37, 93	0
2	B	329/332 (99%)	-0.27	4 (1%) 79 83	12, 16, 33, 51	0
3	C	330/332 (99%)	-0.19	9 (2%) 54 61	10, 15, 36, 82	0
All	All	990/996 (99%)	-0.22	20 (2%) 65 70	10, 17, 36, 93	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	8.0
1	A	96	GLY	6.9
1	A	98	GLU	4.8
1	A	95	GLU	4.8
1	A	332	SER	4.6
3	C	1	MET	4.3
1	A	3	LYS	4.2
3	C	95	GLU	4.2
3	C	98	GLU	3.6
2	B	1	MET	3.4
2	B	3	LYS	3.3
3	C	96	GLY	2.8
2	B	332	SER	2.8
3	C	332	SER	2.8
3	C	2	ALA	2.6
3	C	97	MET	2.6
2	B	204	SER	2.5
1	A	218	ALA	2.3
3	C	101	ASP	2.3
3	C	3	LYS	2.1

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

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(Å ²)	Q<0.9
2	SME	B	97[A]	9/10	0.95	0.14	25,30,33,35	6
2	SME	B	97[B]	9/10	0.95	0.14	25,31,41,41	6
3	SME	C	56[A]	9/10	0.97	0.11	9,11,14,22	6
3	SME	C	56[B]	9/10	0.97	0.11	9,11,20,24	6
2	CSD	B	330[B]	8/9	0.98	0.08	20,26,29,29	5
2	SME	B	56	9/10	0.98	0.09	10,11,25,25	1
2	CSD	B	330[A]	6/9	0.98	0.08	20,22,24,28	3
3	CSO	C	330	7/8	0.99	0.05	23,24,27,28	1

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, 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(Å ²)	Q<0.9
6	GOL	B	406	6/6	0.64	0.25	56,62,70,75	0
10	ETX	A	411	6/6	0.78	0.20	26,27,28,29	6
9	TRS	A	410	8/8	0.80	0.21	43,44,48,50	8
12	EDO	C	412	4/4	0.82	0.13	46,46,46,46	4
8	FMT	C	411	3/3	0.83	0.12	37,37,38,39	3
8	FMT	B	416	3/3	0.83	0.12	46,46,46,47	0
11	ACT	B	414	4/4	0.85	0.12	56,56,57,57	0
6	GOL	B	407	6/6	0.86	0.13	36,40,42,45	0
6	GOL	C	405	6/6	0.87	0.17	39,41,45,45	0
6	GOL	A	405	6/6	0.89	0.17	47,51,52,53	0
8	FMT	B	415	3/3	0.89	0.09	54,54,54,54	0
12	EDO	B	418	4/4	0.90	0.28	26,37,62,62	0
7	PEO	C	409	2/2	0.90	0.14	37,37,37,38	2
8	FMT	A	409	3/3	0.91	0.08	43,43,43,44	0

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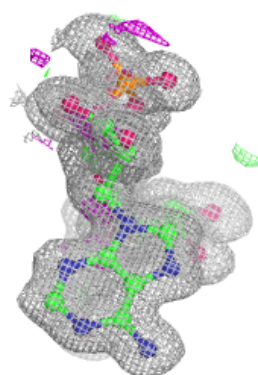
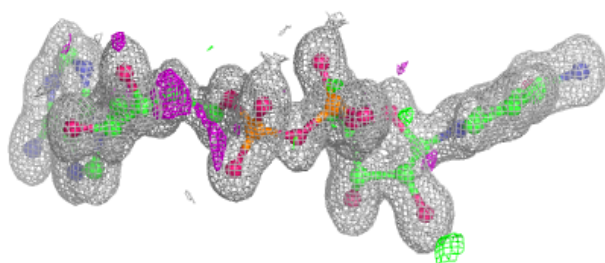
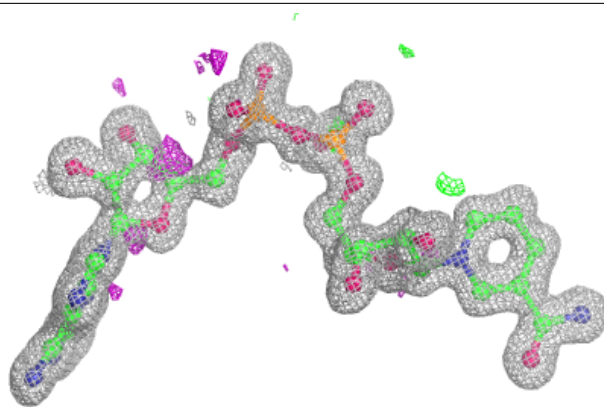
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PEO	C	407	2/2	0.92	0.11	30,30,30,30	2
12	EDO	B	417	4/4	0.92	0.19	22,22,23,27	4
7	PEO	A	408	2/2	0.93	0.11	29,29,29,30	2
7	PEO	B	411	2/2	0.93	0.16	17,17,17,19	2
6	GOL	A	404	6/6	0.94	0.09	19,23,28,30	0
11	ACT	B	412	4/4	0.95	0.08	34,35,35,37	0
11	ACT	B	413	4/4	0.95	0.07	37,37,38,39	0
7	PEO	B	409	2/2	0.96	0.08	31,31,31,31	2
6	GOL	B	405	6/6	0.96	0.08	23,23,28,31	6
8	FMT	C	410	3/3	0.97	0.06	36,36,38,40	0
7	PEO	A	407	2/2	0.97	0.14	18,18,18,21	2
5	SO4	A	403	5/5	0.98	0.09	28,31,34,35	0
5	SO4	C	404	5/5	0.98	0.08	22,23,26,26	5
4	NAD	B	401	44/44	0.98	0.06	12,14,16,19	0
7	PEO	B	410	2/2	0.98	0.12	23,23,23,25	2
4	NAD	C	401	44/44	0.98	0.06	10,13,14,16	0
7	PEO	A	406	2/2	0.98	0.05	17,17,17,17	2
7	PEO	C	408	2/2	0.98	0.11	25,25,25,27	2
5	SO4	C	402	5/5	0.99	0.06	12,14,16,17	5
7	PEO	C	406	2/2	0.99	0.07	17,17,17,19	2
5	SO4	C	403	5/5	0.99	0.07	17,19,21,26	5
5	SO4	A	402	5/5	0.99	0.04	18,18,21,21	0
4	NAD	A	401	44/44	0.99	0.06	11,15,17,18	0
5	SO4	B	402	5/5	0.99	0.05	20,20,23,25	0
7	PEO	B	408	2/2	0.99	0.09	20,20,20,22	2
5	SO4	B	403	5/5	0.99	0.07	18,21,25,27	0
5	SO4	B	404	5/5	0.99	0.05	15,16,18,18	1

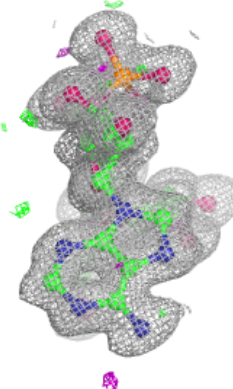
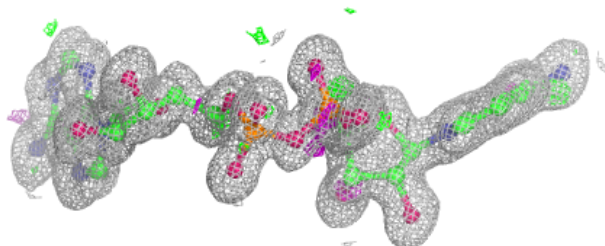
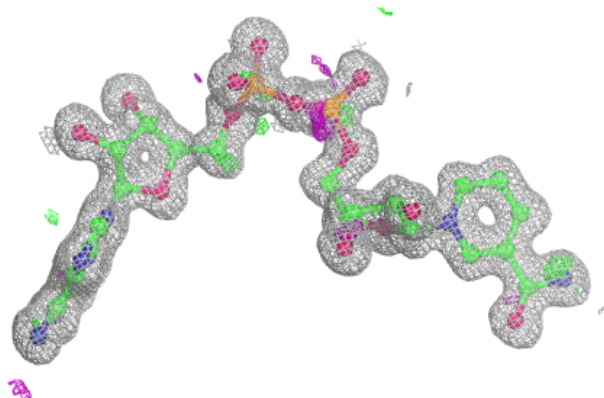
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

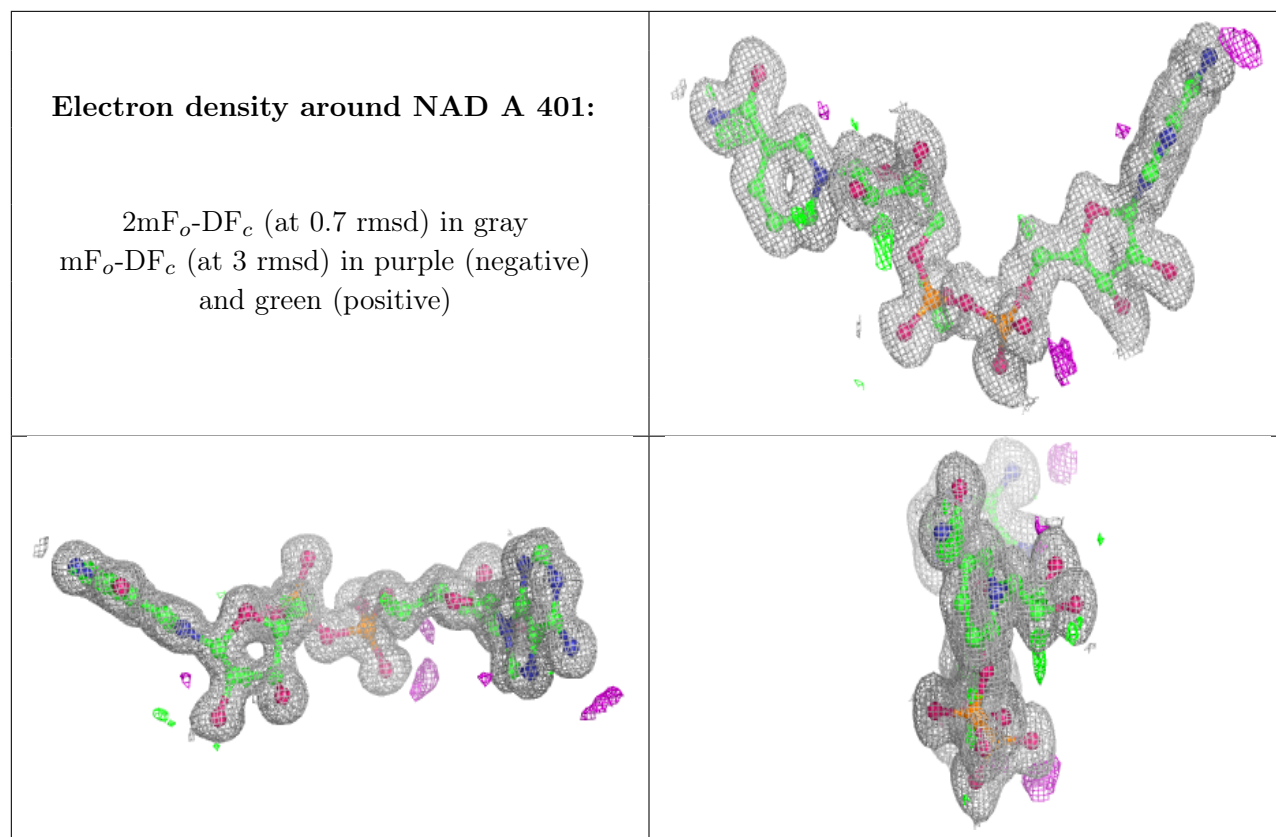
Electron density around NAD B 401:

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

**Electron density around NAD C 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.