



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:57 AM UTC

PDB ID : 6XXJ / pdb_00006xxj
Title : Crystal Structure of Human Deoxyhypusine Synthase in complex with spermidine and NAD
Authors : Wator, E.; Wilk, P.; Grudnik, P.
Deposited on : 2020-01-27
Resolution : 1.41 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 : 4-5-2 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

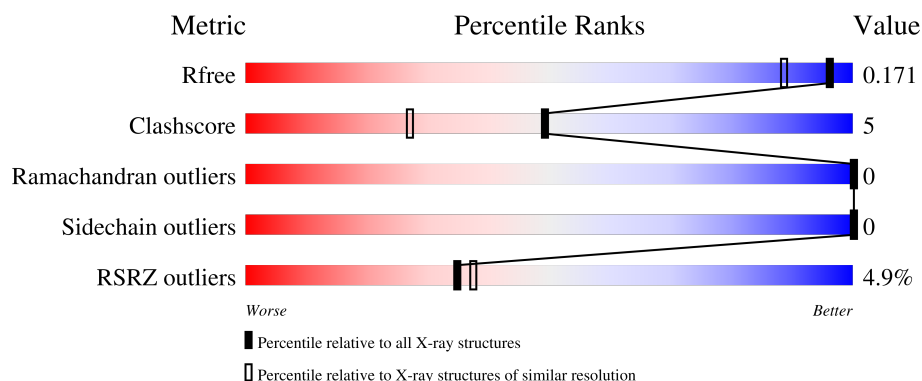
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

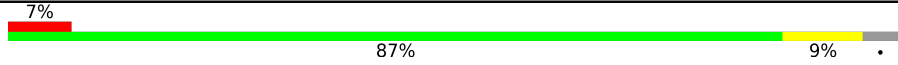
The reported resolution of this entry is 1.41 Å.

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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	369	
1	B	369	

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	SPD	A	401	-	-	X	-
2	SPD	B	401	-	-	X	-
5	ACT	B	411	-	-	X	-
6	BME	A	408	-	-	X	-
7	FMT	A	412	-	-	X	-
7	FMT	A	413	-	-	X	-
7	FMT	B	413	-	-	X	-
9	OXM	B	409	-	X	-	-

2 Entry composition [i](#)

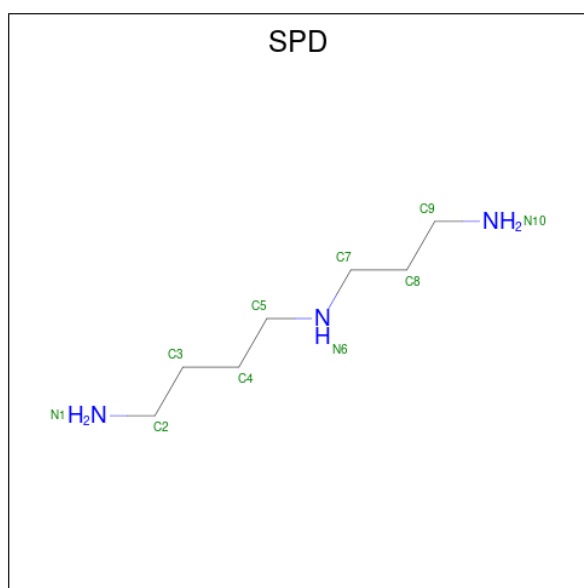
There are 11 unique types of molecules in this entry. The entry contains 6443 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Deoxyhypusine synthase.

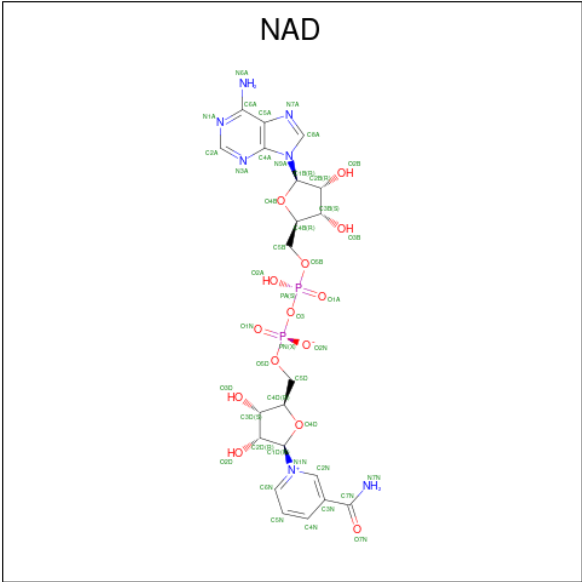
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	19	0
			2869	1832	482	536	19			
1	B	336	Total	C	N	O	S	0	22	0
			2766	1765	465	517	19			

- Molecule 2 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



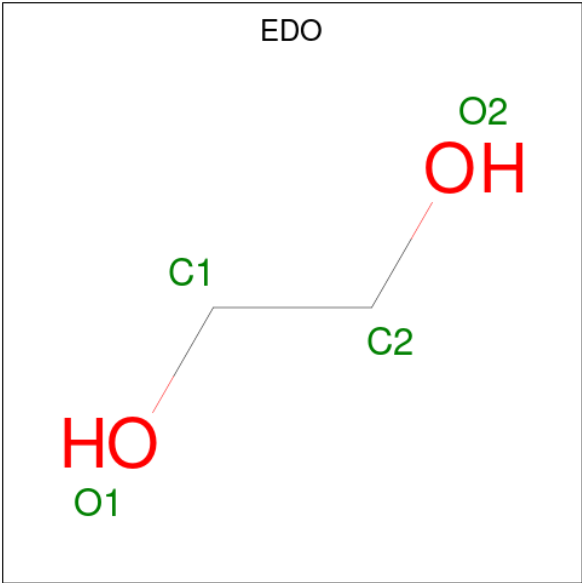
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	7	3		
2	B	1	Total	C	N	0	0
			10	7	3		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



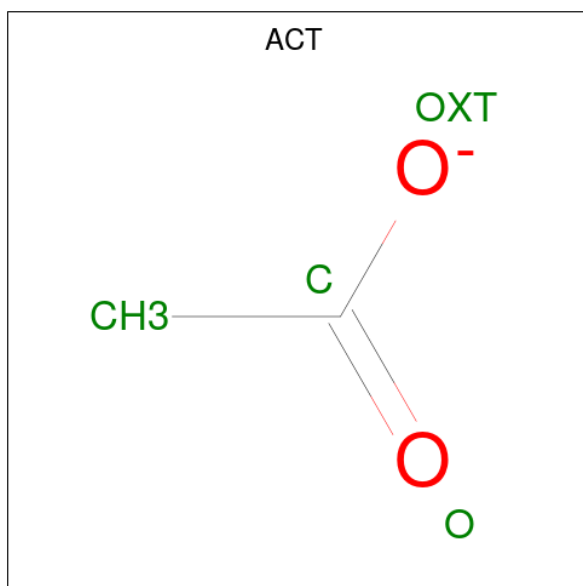
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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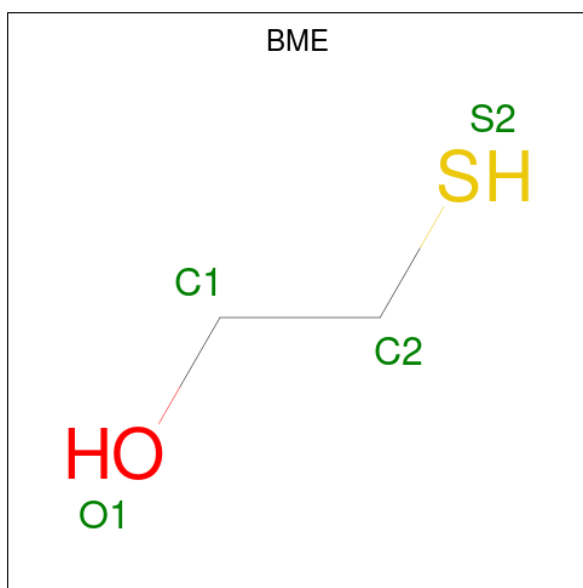
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



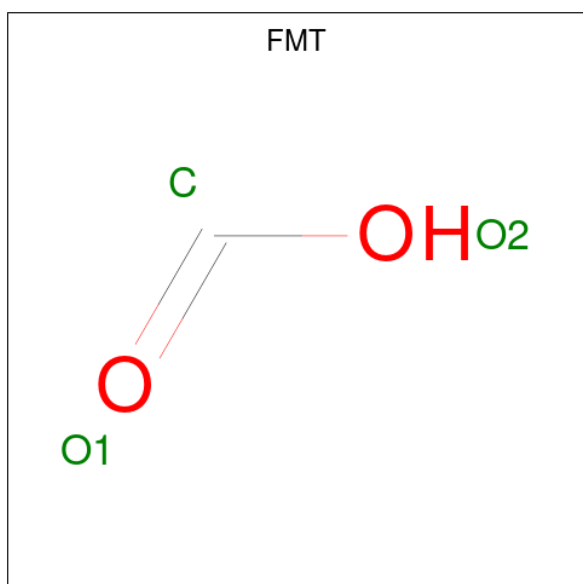
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



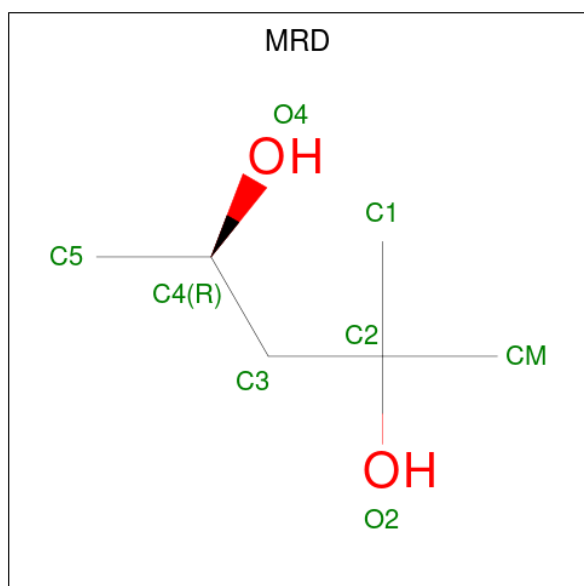
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



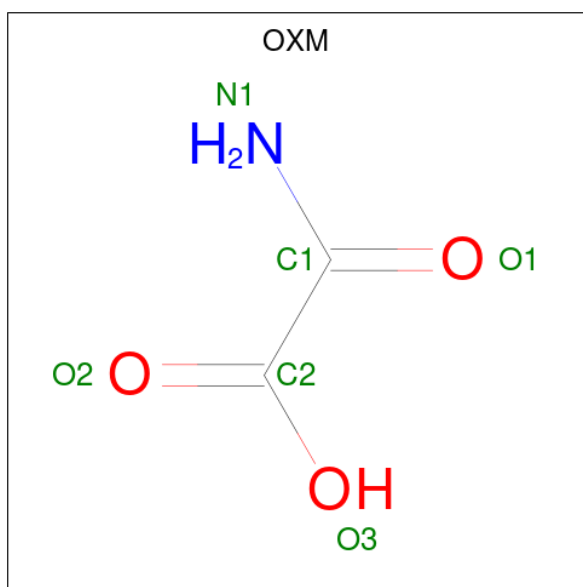
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



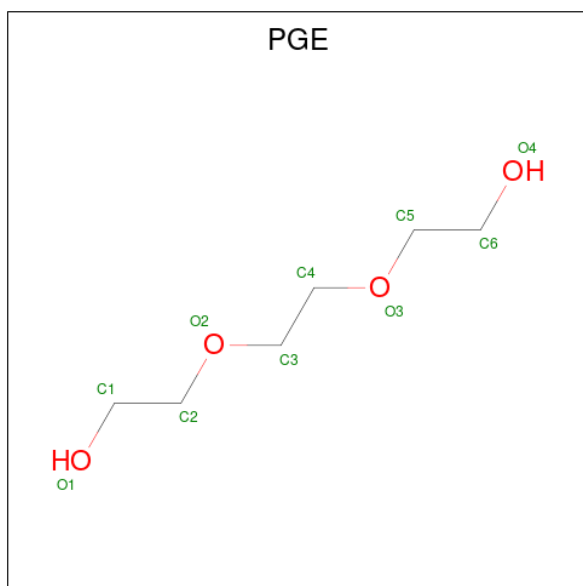
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is OXAMIC ACID (CCD ID: OXM) (formula: C₂H₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

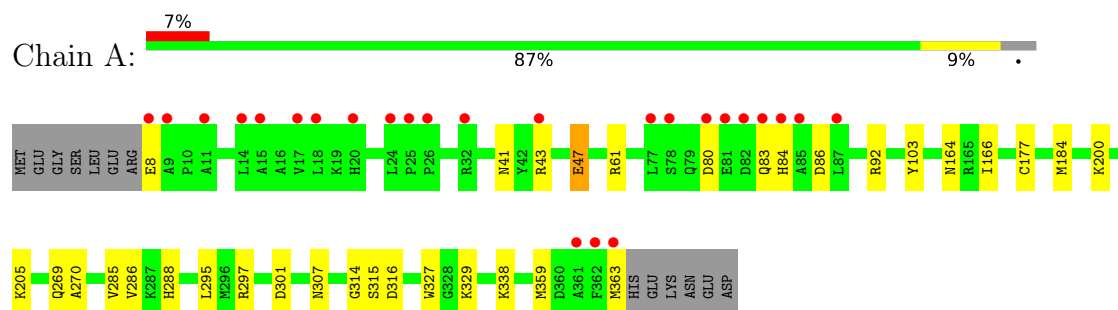
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	319	Total 319	O 319	0	0
11	B	274	Total 274	O 274	0	0

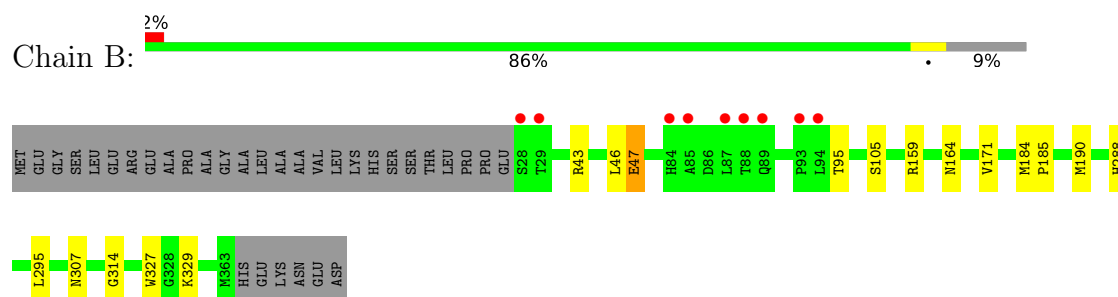
3 Residue-property plots [i](#)

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: Deoxyhypusine synthase



• Molecule 1: Deoxyhypusine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.49Å 105.49Å 160.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.24 – 1.41 46.24 – 1.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.24-1.41) 99.9 (46.24-1.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.41Å)	Xtriage
Refinement program	PHENIX v1.17.1	Depositor
R, R_{free}	0.142 , 0.160 0.159 , 0.171	Depositor DCC
R_{free} test set	2100 reflections (1.06%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6443	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: CSS, PGE, SPD, NAD, BME, EDO, ACT, MRD, FMT, OXM

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	0.60	5/2958 (0.2%)	0.67	0/4014
1	B	0.52	5/2863 (0.2%)	0.71	11/3879 (0.3%)
All	All	0.56	10/5821 (0.2%)	0.69	11/7893 (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
1	A	0	3
1	B	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	GLU	N-CA	7.18	1.55	1.46
1	B	184	MET	C-O	-6.92	1.17	1.24
1	B	190	MET	C-O	-6.24	1.16	1.24
1	B	47	GLU	CA-C	6.19	1.61	1.52
1	A	205	LYS	C-O	-5.54	1.17	1.24
1	B	185	PRO	C-O	-5.28	1.18	1.24
1	A	47	GLU	C-O	-5.26	1.17	1.24
1	A	270	ALA	C-O	-5.23	1.17	1.24
1	A	92	ARG	C-O	-5.07	1.17	1.24
1	A	269	GLN	C-O	-5.03	1.18	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46[A]	LEU	CA-C-O	8.68	129.91	120.10
1	B	46[B]	LEU	CA-C-O	8.68	129.91	120.10
1	B	43[A]	ARG	CA-C-O	7.12	128.10	120.55
1	B	43[B]	ARG	CA-C-O	7.12	128.10	120.55
1	B	47	GLU	CA-C-O	6.92	127.89	119.38
1	B	46[A]	LEU	O-C-N	-6.31	115.43	122.12
1	B	46[B]	LEU	O-C-N	-6.31	115.43	122.12
1	B	43[A]	ARG	N-CA-C	6.21	118.05	111.28
1	B	43[B]	ARG	N-CA-C	6.21	118.05	111.28
1	B	46[A]	LEU	N-CA-C	5.91	117.72	111.28
1	B	46[B]	LEU	N-CA-C	5.91	117.72	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	GLU	Mainchain
1	A	86[A]	ASP	Mainchain
1	A	86[B]	ASP	Mainchain
1	B	47	GLU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2869	0	2855	37	0
1	B	2766	0	2771	17	0
2	A	10	0	19	9	0
2	B	10	0	19	7	0
3	A	44	0	26	1	0
3	B	44	0	26	6	0
4	A	16	0	24	3	0
4	B	20	0	30	0	0
5	A	4	0	3	0	0
5	B	12	0	9	2	0
6	A	16	0	24	5	0
7	A	9	0	3	9	0
7	B	6	0	2	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	8	0	14	0	0
9	B	6	0	2	0	0
10	B	10	0	14	5	0
11	A	319	0	0	4	1
11	B	274	0	0	4	0
All	All	6443	0	5841	63	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 5.

All (63) 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)
2:A:401:SPD:HN12	7:A:413:FMT:C	1.61	1.13
1:B:329:LYS:NZ	2:B:401:SPD:H51	1.76	0.99
4:A:405:EDO:H22	11:A:642:HOH:O	1.67	0.93
1:B:288:HIS:NE2	2:B:401:SPD:H52	1.83	0.92
1:A:184:MET:HE3	11:A:517:HOH:O	1.70	0.91
1:A:288:HIS:NE2	2:A:401:SPD:H52	1.85	0.91
1:A:166:ILE:HG23	7:B:413:FMT:H	1.51	0.90
1:A:43[A]:ARG:NH2	1:A:47:GLU:OE1	2.07	0.87
1:A:177:CSS:SD	11:A:699:HOH:O	2.31	0.87
2:A:401:SPD:N1	7:A:413:FMT:C	2.41	0.83
1:B:329:LYS:HZ1	2:B:401:SPD:H51	1.43	0.82
1:B:329:LYS:HZ3	2:B:401:SPD:H51	1.45	0.80
1:A:80:ASP:CG	1:A:83:GLN:HG2	2.05	0.80
1:A:359:MET:HE2	1:A:363:MET:SD	2.24	0.78
1:A:329:LYS:NZ	2:A:401:SPD:H51	1.99	0.77
1:A:166:ILE:CG2	7:B:413:FMT:H	2.17	0.73
2:B:401:SPD:HN12	7:B:413:FMT:C	2.02	0.73
7:A:412:FMT:H	1:B:159:ARG:HE	1.53	0.72
1:A:338:LYS:H	6:A:408:BME:H12	1.59	0.67
1:A:166:ILE:HG23	7:B:413:FMT:C	2.23	0.67
7:A:412:FMT:C	1:B:159:ARG:HE	2.08	0.66
1:A:329:LYS:HZ1	2:A:401:SPD:H51	1.62	0.65
1:A:316:ASP:N	7:A:413:FMT:H	2.12	0.65
1:B:329:LYS:HZ3	2:B:401:SPD:C5	2.12	0.62
1:A:329:LYS:HZ3	2:A:401:SPD:H51	1.67	0.60
1:A:315:SER:C	7:A:413:FMT:H	2.28	0.58
1:A:316:ASP:HA	7:A:413:FMT:H	1.86	0.57
1:B:164:ASN:HB2	1:B:171[B]:VAL:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ASP:CA	7:A:413:FMT:H	2.35	0.56
1:B:314:GLY:O	7:B:413:FMT:C	2.55	0.55
4:A:405:EDO:C2	11:A:642:HOH:O	2.43	0.51
1:A:80:ASP:CB	1:A:83:GLN:HG2	2.41	0.50
1:A:41:ASN:HD21	1:A:43[B]:ARG:HH11	1.60	0.49
10:B:415:PGE:H6	11:B:507:HOH:O	2.14	0.47
10:B:415:PGE:C6	11:B:507:HOH:O	2.62	0.47
1:A:297:ARG:NH1	1:A:301:ASP:OD1	2.48	0.46
1:A:80:ASP:HB3	1:A:83:GLN:OE1	2.15	0.46
5:B:411:ACT:H3	10:B:415:PGE:O2	2.15	0.46
1:A:359:MET:O	1:A:359:MET:HE3	2.15	0.46
5:B:411:ACT:CH3	10:B:415:PGE:O2	2.63	0.46
1:A:61:ARG:HH12	6:A:408:BME:HO1	1.62	0.46
1:A:314:GLY:O	7:A:413:FMT:C	2.64	0.45
1:A:327:TRP:CE2	1:B:164:ASN:HB3	2.52	0.45
1:A:338:LYS:H	6:A:408:BME:C1	2.26	0.45
1:A:103:TYR:N	1:A:286[A]:VAL:HG11	2.31	0.44
1:B:307:ASN:HA	3:B:404:NAD:H2A	1.99	0.44
1:A:80:ASP:OD2	1:A:83:GLN:HG2	2.17	0.44
1:A:315:SER:HB3	3:B:404:NAD:C8A	2.49	0.43
1:A:83:GLN:HG3	1:A:84:HIS:N	2.33	0.43
1:B:95:THR:HG23	11:B:556:HOH:O	2.18	0.43
1:A:164:ASN:HB3	1:B:327:TRP:CE2	2.55	0.41
1:A:307:ASN:HA	3:A:402:NAD:H2A	2.02	0.41
6:A:409:BME:S2	1:B:295:LEU:HD21	2.61	0.41
1:B:105[C]:SER:OG	3:B:404:NAD:C7N	2.68	0.41
1:A:288:HIS:NE2	2:A:401:SPD:C5	2.72	0.41
1:A:295:LEU:HD23	2:A:401:SPD:H101	1.85	0.41
1:A:338:LYS:N	6:A:408:BME:H12	2.29	0.41
1:B:295:LEU:HD23	2:B:401:SPD:H101	1.85	0.41
1:B:307:ASN:HA	3:B:404:NAD:C2A	2.50	0.41
1:A:200:LYS:HA	4:A:405:EDO:H11	2.03	0.40
10:B:415:PGE:H4	11:B:741:HOH:O	2.21	0.40
1:A:285[B]:VAL:HG12	3:B:404:NAD:O3D	2.22	0.40
2:A:401:SPD:H41	3:B:404:NAD:C3N	2.52	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)
11:A:653:HOH:O	11:A:756:HOH:O[6_444]	2.14	0.06

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	372/369 (101%)	366 (98%)	6 (2%)	0	100	100
1	B	356/369 (96%)	353 (99%)	3 (1%)	0	100	100
All	All	728/738 (99%)	719 (99%)	9 (1%)	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	309/309 (100%)	309 (100%)	0	100	100
1	B	303/309 (98%)	303 (100%)	0	100	100
All	All	612/618 (99%)	612 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	161	ASN
1	A	269	GLN
1	B	37	ASN
1	B	228	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSS	B	177	1	4,6,7	0.94	0	2,6,8	0.56	0
1	CSS	A	177	1	4,6,7	0.98	0	2,6,8	0.18	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
1	CSS	B	177	1	-	0/1/5/7	-
1	CSS	A	177	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	177	CSS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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	BME	A	409	-	3,3,3	0.25	0	2,2,2	0.90	0
4	EDO	A	405	-	3,3,3	0.45	0	2,2,2	0.25	0
6	BME	A	410	-	3,3,3	0.28	0	2,2,2	0.52	0
2	SPD	B	401	-	9,9,9	0.40	0	8,8,8	0.48	0
7	FMT	A	412	-	2,2,2	0.79	0	1,1,1	0.59	0
10	PGE	B	415	-	9,9,9	0.34	0	8,8,8	0.71	0
7	FMT	B	413	-	2,2,2	0.54	0	1,1,1	0.79	0
6	BME	A	411	-	3,3,3	0.34	0	2,2,2	0.78	0
5	ACT	B	411	-	3,3,3	0.91	0	3,3,3	0.76	0
5	ACT	B	410	-	3,3,3	0.98	0	3,3,3	0.87	0
5	ACT	B	412	-	3,3,3	0.96	0	3,3,3	0.85	0
4	EDO	B	405	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.33	0
5	ACT	A	407	-	3,3,3	0.97	0	3,3,3	0.84	0
4	EDO	B	407	-	3,3,3	0.48	0	2,2,2	0.46	0
3	NAD	A	402	-	46,48,48	1.28	5 (10%)	64,73,73	1.89	15 (23%)
2	SPD	A	401	-	9,9,9	0.45	0	8,8,8	0.52	0
9	OXM	B	409	-	5,5,5	2.62	3 (60%)	2,6,6	1.26	0
3	NAD	B	404	-	46,48,48	1.31	6 (13%)	64,73,73	1.84	19 (29%)
7	FMT	B	414	-	2,2,2	0.15	0	1,1,1	0.17	0
4	EDO	B	408	-	3,3,3	0.22	0	2,2,2	0.37	0
7	FMT	A	414	-	2,2,2	0.25	0	1,1,1	0.06	0
8	MRD	B	403	-	7,7,7	0.74	0	9,10,10	0.39	0
6	BME	A	408	-	3,3,3	0.64	0	2,2,2	0.72	0
4	EDO	B	406	-	3,3,3	0.42	0	2,2,2	0.38	0
7	FMT	A	413	-	2,2,2	0.15	0	1,1,1	0.03	0
4	EDO	A	406	-	3,3,3	0.45	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	402	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BME	A	409	-	-	0/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
6	BME	A	410	-	-	0/1/1/1	-
2	SPD	B	401	-	-	4/7/7/7	-
10	PGE	B	415	-	-	3/7/7/7	-
6	BME	A	411	-	-	1/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	407	-	-	1/1/1/1	-
3	NAD	A	402	-	-	5/30/62/62	0/5/5/5
2	SPD	A	401	-	-	4/7/7/7	-
3	NAD	B	404	-	-	5/30/62/62	0/5/5/5
4	EDO	B	408	-	-	0/1/1/1	-
8	MRD	B	403	-	-	0/5/5/5	-
6	BME	A	408	-	-	1/1/1/1	-
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
9	OXM	B	409	-	-	4/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	NAD	C5A-C4A	4.36	1.46	1.39
9	B	409	OXM	C1-N1	4.22	1.45	1.33
3	A	402	NAD	C5A-C4A	4.14	1.46	1.39
3	B	404	NAD	C5A-N7A	-2.66	1.34	1.39
3	B	404	NAD	C5A-C6A	2.65	1.48	1.41
3	B	404	NAD	C2N-N1N	-2.56	1.32	1.35
3	A	402	NAD	PA-O3	2.52	1.62	1.59
9	B	409	OXM	C1-C2	-2.47	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	409	OXM	O1-C1	-2.35	1.18	1.24
3	A	402	NAD	C5A-N7A	-2.32	1.34	1.39
3	A	402	NAD	C8A-N7A	2.26	1.36	1.31
3	A	402	NAD	O4D-C1D	2.18	1.43	1.40
3	B	404	NAD	C8A-N9A	-2.11	1.34	1.37
3	B	404	NAD	PA-O3	2.01	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAD	C5A-C4A-N3A	-5.50	119.15	126.72
3	B	404	NAD	C5A-C4A-N3A	-5.31	119.41	126.72
3	A	402	NAD	N3A-C4A-N9A	4.90	135.50	127.17
3	A	402	NAD	O3-PN-O1N	-4.46	97.29	110.70
3	B	404	NAD	C4A-C5A-N7A	-4.39	105.56	110.58
3	A	402	NAD	N3A-C2A-N1A	-4.32	122.05	128.58
3	A	402	NAD	O4B-C1B-N9A	3.89	115.57	108.09
3	B	404	NAD	N3A-C4A-N9A	3.87	133.75	127.17
3	A	402	NAD	C2A-N3A-C4A	3.59	120.59	111.83
3	A	402	NAD	O2N-PN-O1N	3.31	127.82	112.44
3	B	404	NAD	C5A-N7A-C8A	3.30	108.63	103.45
3	A	402	NAD	C2B-C1B-N9A	-3.26	105.20	113.30
3	B	404	NAD	O3-PN-O1N	-3.14	101.24	110.70
3	B	404	NAD	O2A-PA-O3	3.14	115.76	107.27
3	A	402	NAD	C4A-N9A-C8A	3.09	108.98	105.74
3	B	404	NAD	C2A-N1A-C6A	3.06	123.76	118.73
3	B	404	NAD	C2B-C1B-N9A	-3.06	105.71	113.30
3	B	404	NAD	N3A-C2A-N1A	-3.02	124.01	128.58
3	B	404	NAD	O4B-C1B-N9A	3.02	113.88	108.09
3	B	404	NAD	O2N-PN-O1N	2.88	125.85	112.44
3	B	404	NAD	C2A-N3A-C4A	2.80	118.67	111.83
3	A	402	NAD	O3-PA-O1A	-2.64	102.77	110.70
3	A	402	NAD	C2A-N1A-C6A	2.50	122.83	118.73
3	B	404	NAD	C3B-C2B-C1B	2.44	106.08	101.46
3	A	402	NAD	C4A-C5A-N7A	-2.42	107.82	110.58
3	B	404	NAD	O2D-C2D-C3D	2.41	119.54	111.82
3	A	402	NAD	C3B-C2B-C1B	2.32	105.85	101.46
3	B	404	NAD	C6N-N1N-C2N	2.27	123.81	121.88
3	B	404	NAD	O2A-PA-O1A	2.26	122.97	112.44
3	B	404	NAD	O3-PA-O1A	-2.19	104.12	110.70
3	B	404	NAD	C4A-N9A-C8A	2.18	108.02	105.74
3	B	404	NAD	N9A-C8A-N7A	-2.11	110.95	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAD	C4B-O4B-C1B	2.09	114.09	109.47
3	A	402	NAD	O2A-PA-O3	2.05	112.81	107.27

There are no chirality outliers.

All (32) torsion outliers are listed below:

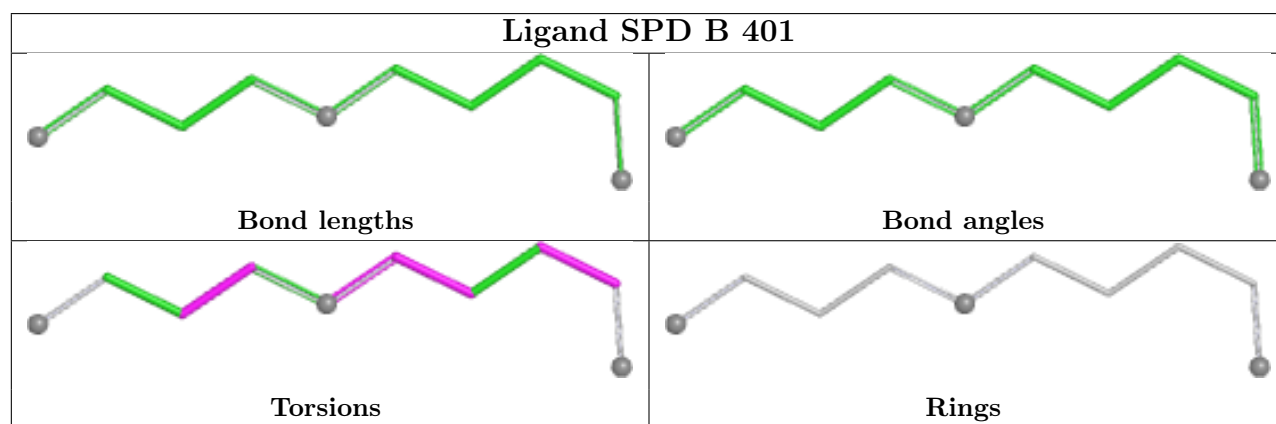
Mol	Chain	Res	Type	Atoms
3	A	402	NAD	C5D-O5D-PN-O3
3	A	402	NAD	C5D-O5D-PN-O1N
3	B	404	NAD	C5D-O5D-PN-O3
3	B	404	NAD	C5D-O5D-PN-O1N
9	B	409	OXM	N1-C1-C2-O2
9	B	409	OXM	N1-C1-C2-O3
9	B	409	OXM	O1-C1-C2-O2
9	B	409	OXM	O1-C1-C2-O3
2	B	401	SPD	C3-C4-C5-N6
10	B	415	PGE	O2-C3-C4-O3
2	A	401	SPD	C3-C4-C5-N6
10	B	415	PGE	O3-C5-C6-O4
2	B	401	SPD	C4-C5-N6-C7
6	A	408	BME	O1-C1-C2-S2
6	A	411	BME	O1-C1-C2-S2
4	A	403	EDO	O1-C1-C2-O2
4	B	406	EDO	O1-C1-C2-O2
4	A	406	EDO	O1-C1-C2-O2
3	A	402	NAD	PA-O3-PN-O5D
10	B	415	PGE	C1-C2-O2-C3
2	A	401	SPD	C4-C5-N6-C7
3	A	402	NAD	C5D-O5D-PN-O2N
3	B	404	NAD	C5D-O5D-PN-O2N
2	B	401	SPD	N6-C7-C8-C9
2	A	401	SPD	N1-C2-C3-C4
2	B	401	SPD	N1-C2-C3-C4
4	B	407	EDO	O1-C1-C2-O2
3	B	404	NAD	PA-O3-PN-O2N
3	B	404	NAD	PA-O3-PN-O5D
2	A	401	SPD	C8-C7-N6-C5
3	A	402	NAD	PN-O3-PA-O1A
4	A	405	EDO	O1-C1-C2-O2

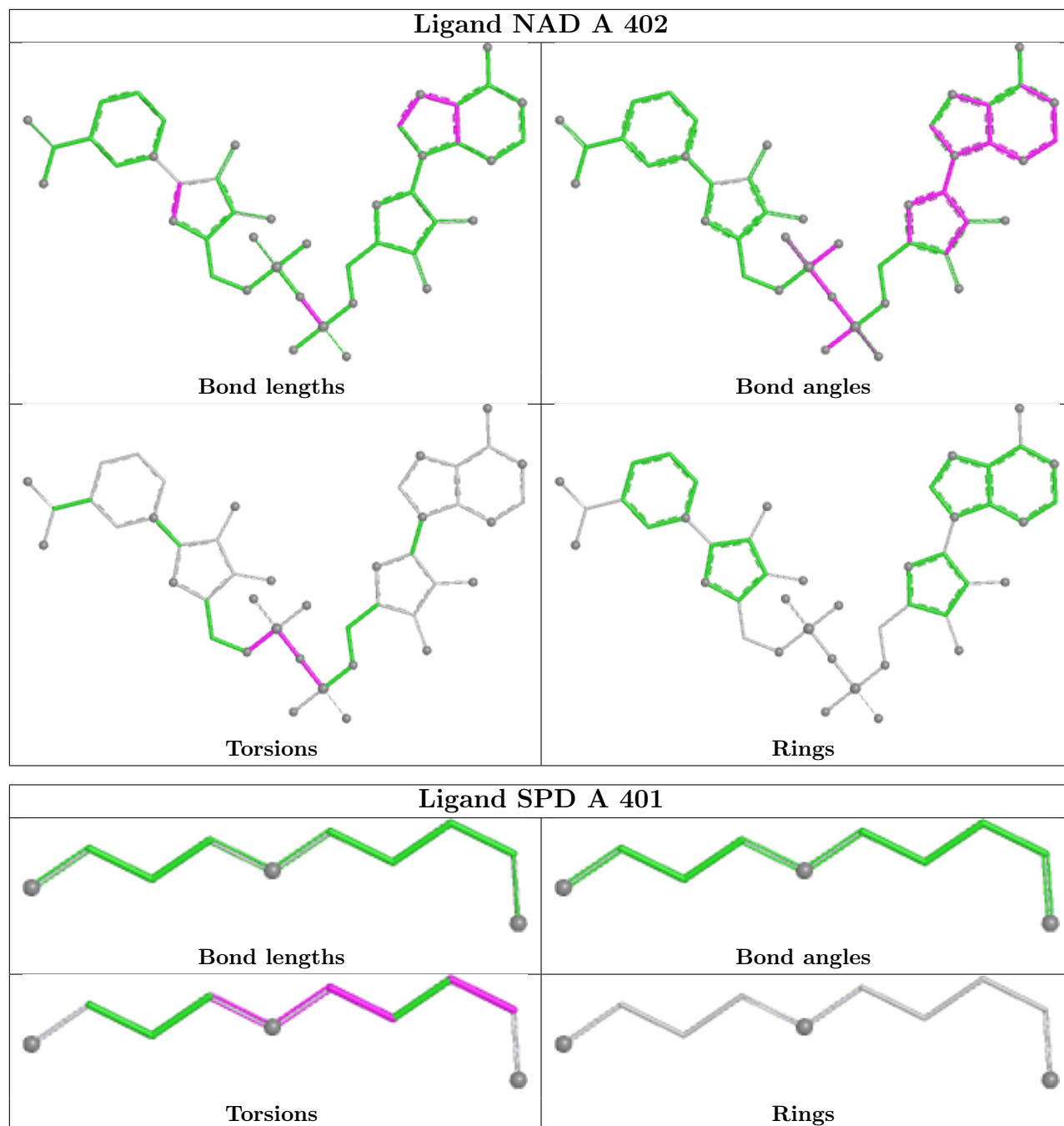
There are no ring outliers.

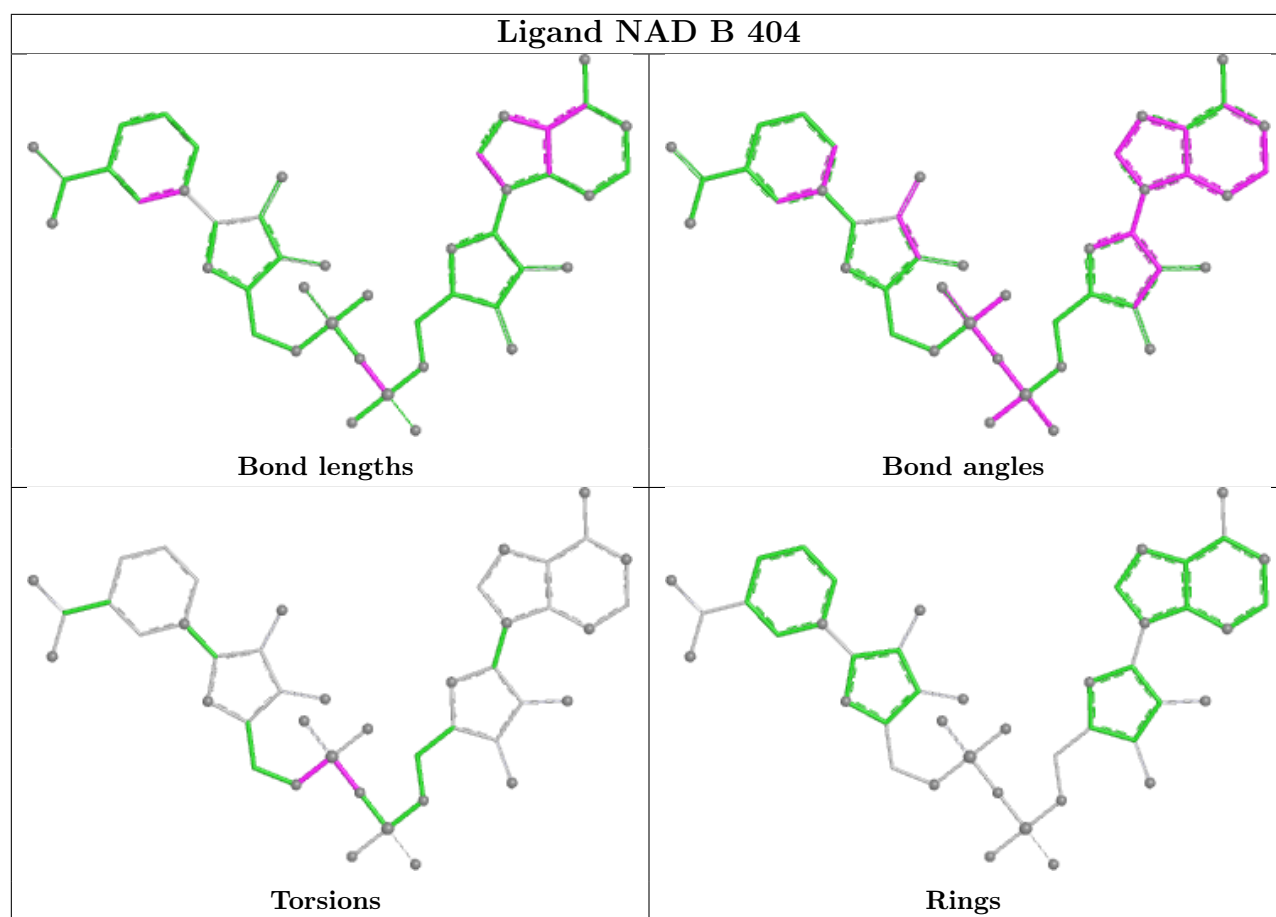
12 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	409	BME	1	0
4	A	405	EDO	3	0
2	B	401	SPD	7	0
7	A	412	FMT	2	0
10	B	415	PGE	5	0
7	B	413	FMT	5	0
5	B	411	ACT	2	0
3	A	402	NAD	1	0
2	A	401	SPD	9	0
3	B	404	NAD	6	0
6	A	408	BME	4	0
7	A	413	FMT	7	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	355/369 (96%)	0.10	25 (7%) 22 25	9, 23, 57, 121	21 (5%)
1	B	335/369 (90%)	-0.07	9 (2%) 56 59	11, 23, 44, 83	23 (6%)
All	All	690/738 (93%)	0.01	34 (4%) 35 37	9, 23, 49, 121	44 (6%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	GLU	9.3
1	A	78	SER	5.6
1	A	363	MET	4.8
1	A	82	ASP	4.3
1	A	9	ALA	3.9
1	B	89	GLN	3.7
1	A	84	HIS	3.7
1	A	43[A]	ARG	3.6
1	A	85	ALA	3.6
1	A	14	LEU	3.6
1	B	94	LEU	3.6
1	A	26	PRO	3.5
1	A	77	LEU	3.5
1	B	28	SER	3.5
1	A	362	PHE	3.2
1	A	361	ALA	3.2
1	B	93	PRO	3.1
1	B	85	ALA	3.1
1	A	32[A]	ARG	3.0
1	A	81	GLU	3.0
1	A	80	ASP	2.9
1	A	18	LEU	2.6
1	B	87	LEU	2.6
1	B	88	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	2.5
1	A	11	ALA	2.3
1	A	25	PRO	2.3
1	A	20	HIS	2.3
1	A	24	LEU	2.2
1	A	83	GLN	2.1
1	B	84	HIS	2.1
1	A	17	VAL	2.1
1	A	15	ALA	2.1
1	B	29	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	CSS	A	177	7/8	0.95	0.10	20,24,33,50	0
1	CSS	B	177	7/8	0.97	0.08	29,32,47,95	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
5	ACT	B	410	4/4	0.71	0.27	63,67,67,69	0
5	ACT	B	412	4/4	0.73	0.28	82,82,83,84	0
6	BME	A	408	4/4	0.73	0.30	74,77,79,80	0
7	FMT	A	412	3/3	0.74	0.22	50,50,53,56	3
4	EDO	A	406	4/4	0.75	0.27	65,67,67,68	4
10	PGE	B	415	10/10	0.75	0.29	70,71,76,77	10

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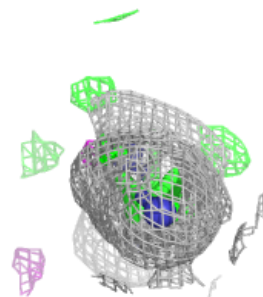
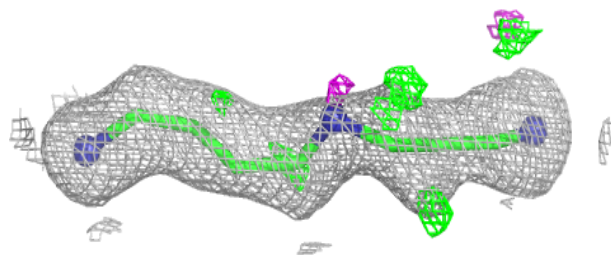
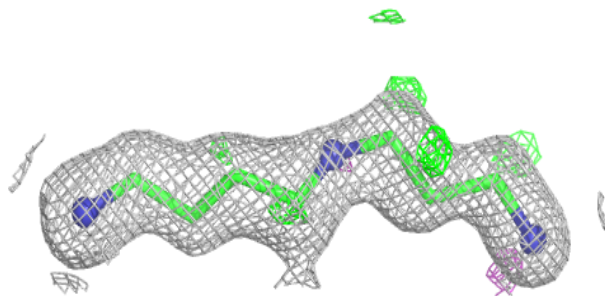
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	B	411	4/4	0.78	0.20	71,72,72,73	0
4	EDO	A	403	4/4	0.81	0.21	89,90,90,90	0
4	EDO	B	406	4/4	0.81	0.20	70,70,71,72	0
4	EDO	B	408	4/4	0.83	0.26	80,80,81,81	0
5	ACT	A	407	4/4	0.83	0.20	87,87,87,87	0
4	EDO	B	405	4/4	0.85	0.17	68,68,68,68	0
9	OXM	B	409	6/6	0.85	0.16	68,72,72,73	0
4	EDO	B	407	4/4	0.85	0.22	38,39,40,41	4
4	EDO	A	404	4/4	0.86	0.22	98,98,98,99	0
7	FMT	B	414	3/3	0.88	0.17	66,66,67,68	0
6	BME	A	411	4/4	0.88	0.19	74,77,79,79	0
4	EDO	A	405	4/4	0.88	0.20	39,40,41,42	4
7	FMT	A	414	3/3	0.89	0.15	52,52,57,59	0
6	BME	A	410	4/4	0.89	0.16	50,54,57,62	4
6	BME	A	409	4/4	0.91	0.15	43,43,44,46	4
2	SPD	B	401	10/10	0.93	0.12	26,34,41,42	0
7	FMT	B	413	3/3	0.94	0.17	20,20,23,24	3
2	SPD	A	401	10/10	0.94	0.11	29,35,40,41	0
7	FMT	A	413	3/3	0.94	0.18	26,26,30,31	3
3	NAD	B	404	44/44	0.94	0.09	20,26,32,38	0
4	EDO	B	402	4/4	0.95	0.12	39,41,44,46	4
3	NAD	A	402	44/44	0.97	0.06	17,20,28,38	0
8	MRD	B	403	8/8	0.97	0.08	32,34,35,36	8

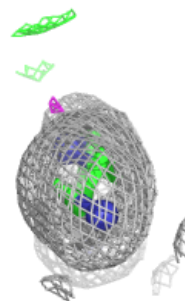
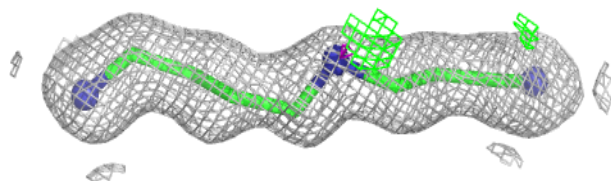
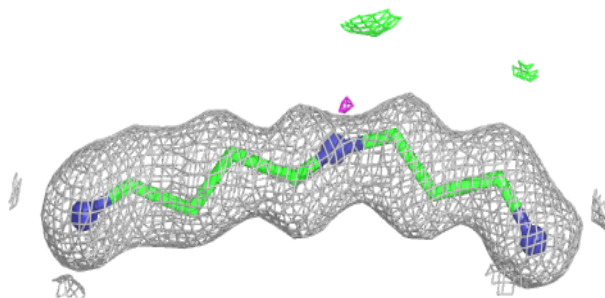
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SPD 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)

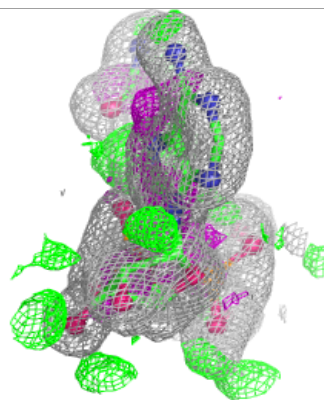
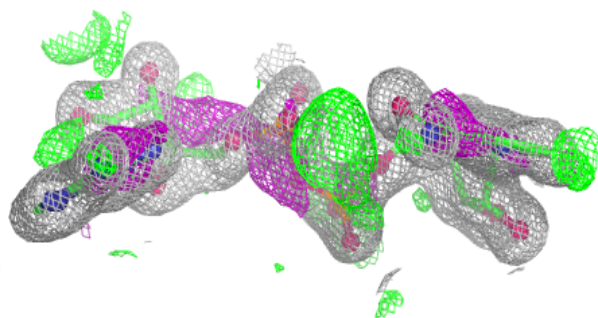
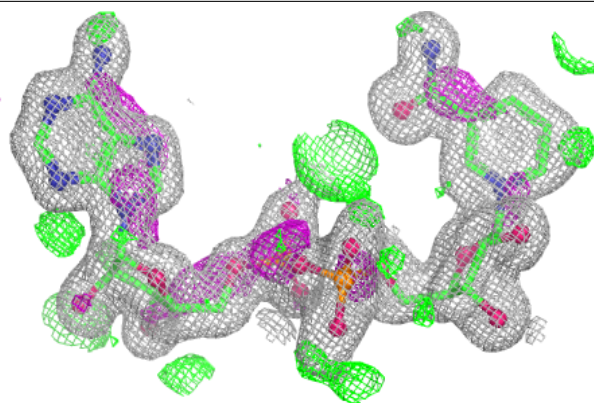
**Electron density around SPD A 401:**

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

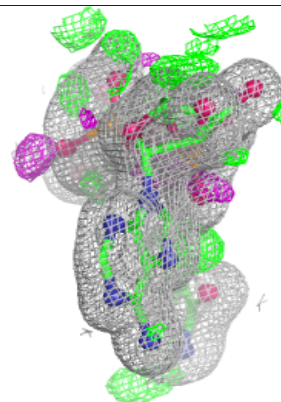
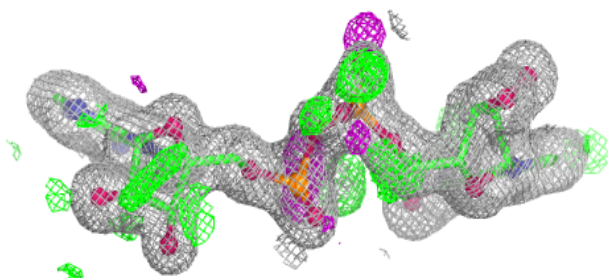
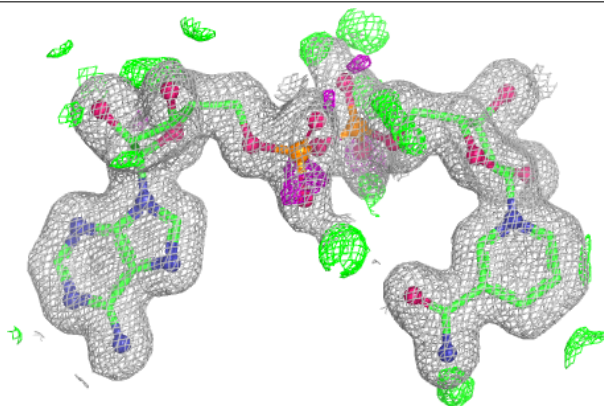


Electron density around NAD B 404:

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

**Electron density around NAD A 402:**

$2mF_o-DF_c$ (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.