



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:48 am BST

PDB ID : 6XXI
Title : Crystal Structure of Human Deoxyhypusine Synthase in complex with NAD
Authors : Wator, E.; Wilk, P.; Grudnik, P.
Deposited on : 2020-01-27
Resolution : 1.68 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 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 : 2.11
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) : 2.11

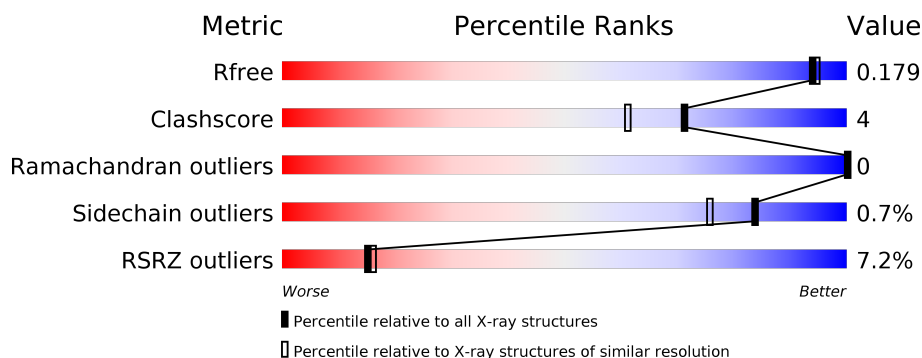
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 on 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	<div> <div>5%</div> <div>83%</div> <div>6%</div> <div>11%</div> </div>
1	B	369	<div> <div>8%</div> <div>86%</div> <div>5%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	1109	-	-	X	-
2	ACT	A	1111	-	-	X	-
3	EDO	B	1504	-	-	-	X
3	EDO	B	1517	-	-	X	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11429 atoms, of which 5513 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	330	Total	C	H	N	O	S	0	11	0
			5253	1676	2619	450	491	17			
1	B	337	Total	C	H	N	O	S	0	10	0
			5336	1700	2653	458	508	17			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



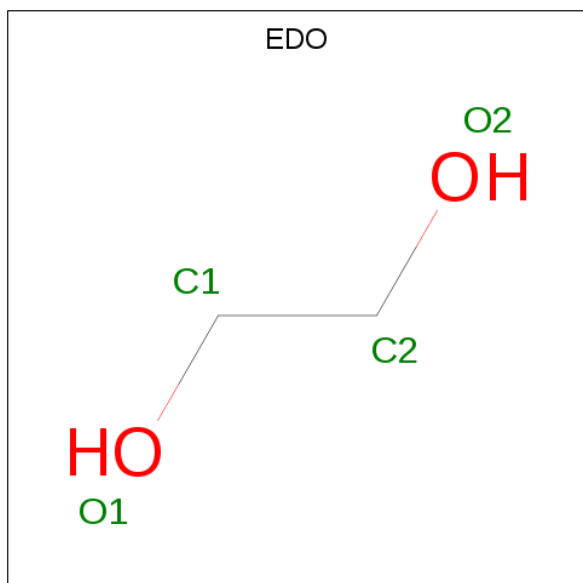
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



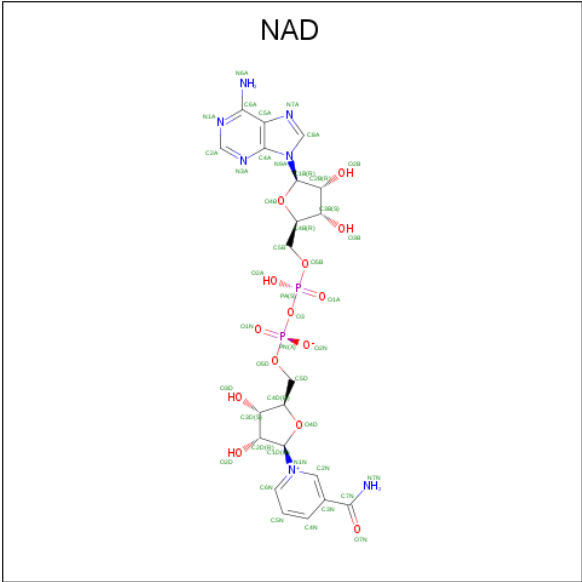
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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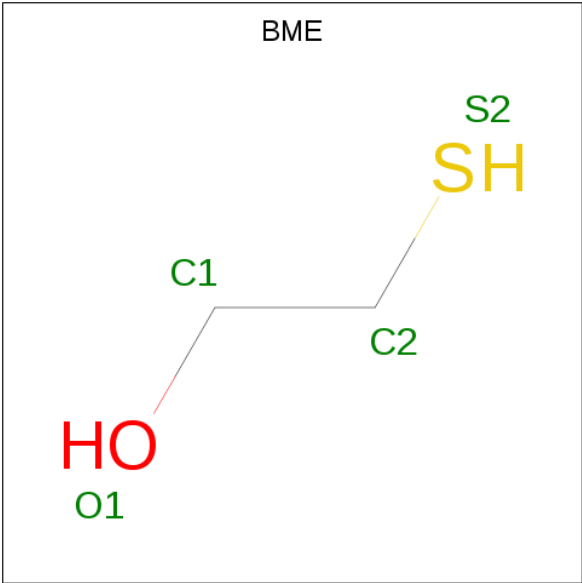
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
4	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



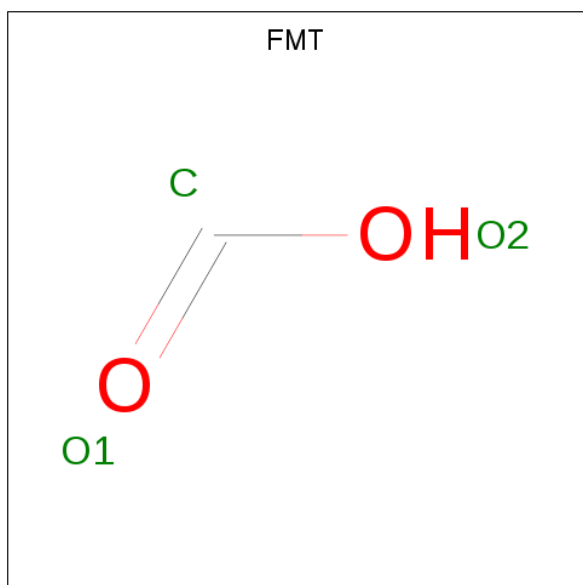
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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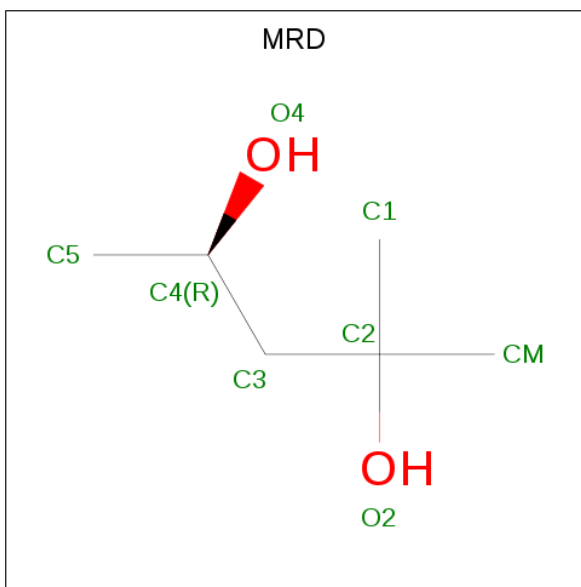
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
5	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			22	6	14	2		

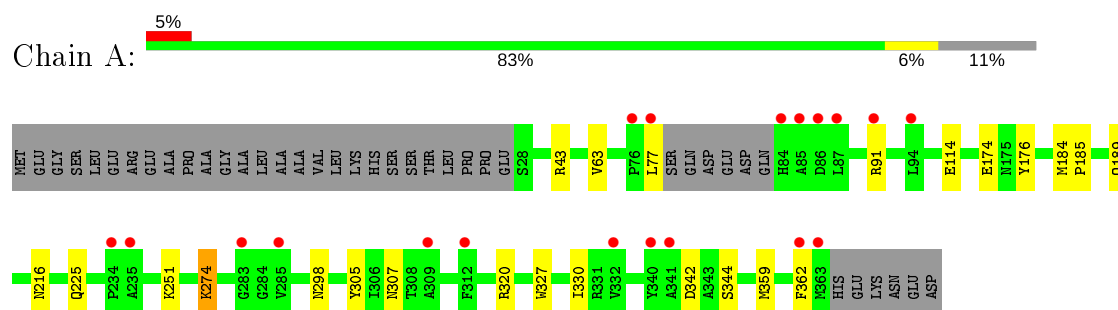
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	181	Total	O	0	0
			181	181		
8	B	175	Total	O	0	0
			175	175		

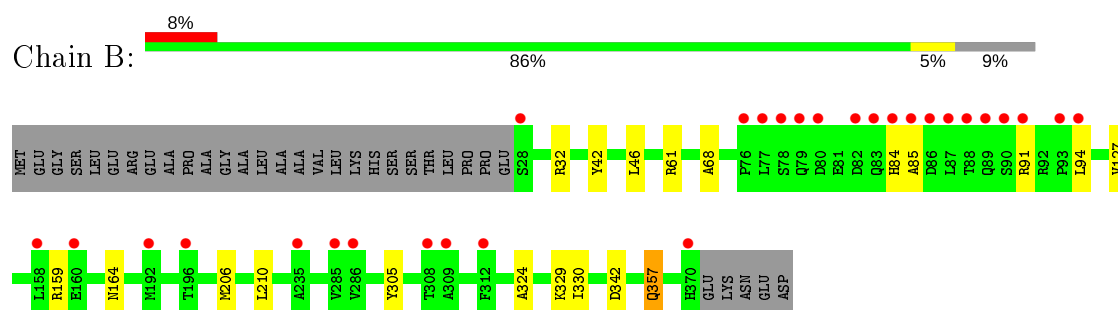
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	104.82Å 104.82Å 160.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.09 – 1.68 46.09 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.09-1.68) 99.7 (46.09-1.68)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.68Å)	Xtriage
Refinement program	PHENIX v.1.17.1	Depositor
R, R_{free}	0.154 , 0.166 0.167 , 0.179	Depositor DCC
R_{free} test set	2100 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11429	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, BME, FMT, EDO, ACT, MRD, CSS

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	1.02	4/2717 (0.1%)	0.91	7/3681 (0.2%)
1	B	0.86	1/2760 (0.0%)	0.83	5/3739 (0.1%)
All	All	0.94	5/5477 (0.1%)	0.87	12/7420 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	PHE	C-N	-16.93	0.95	1.34
1	A	114	GLU	CB-CG	-6.89	1.39	1.52
1	A	114	GLU	CG-CD	6.63	1.61	1.51
1	A	344	SER	CB-OG	5.81	1.49	1.42
1	B	127	VAL	CB-CG1	5.56	1.64	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	LYS	CD-CE-NZ	12.53	140.52	111.70
1	A	362	PHE	O-C-N	10.14	138.93	122.70
1	A	362	PHE	CA-C-N	-7.17	101.42	117.20
1	A	362	PHE	C-N-CA	-6.86	104.54	121.70
1	A	43	ARG	CA-CB-CG	-5.99	100.23	113.40
1	A	342	ASP	CB-CG-OD1	5.84	123.55	118.30
1	B	61[A]	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	61[B]	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	61[A]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	61[B]	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	320	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	342	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2619	2593	19	0
1	B	2683	2653	2620	18	0
2	A	28	21	21	9	0
2	B	28	21	21	0	0
3	A	40	60	58	6	0
3	B	32	48	48	8	0
4	A	44	26	26	1	0
4	B	44	26	26	0	0
5	A	12	18	18	2	0
5	B	4	6	6	0	0
6	A	3	1	1	0	0
7	B	8	14	14	0	0
8	A	181	0	0	4	0
8	B	175	0	0	2	0
All	All	5916	5513	5452	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:HD3	3:B:1517:EDO:H12	1.21	1.18
1:B:32:ARG:HD3	3:B:1517:EDO:C1	1.72	1.16
1:B:32:ARG:CD	3:B:1517:EDO:H12	1.79	1.11
1:A:216:ASN:HD22	2:A:1111:ACT:H1	1.14	1.07
1:B:32:ARG:CG	3:B:1517:EDO:H12	1.94	0.98
1:A:216:ASN:HD22	2:A:1111:ACT:CH3	1.85	0.90
1:A:174:GLU:HB3	3:A:1119:EDO:H12	1.57	0.87
1:B:32:ARG:HD3	3:B:1517:EDO:O1	1.77	0.84
1:B:32:ARG:HG2	3:B:1517:EDO:H12	1.75	0.69
1:B:42:TYR:O	1:B:46[B]:LEU:HD13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLN:HA	3:A:1113:EDO:O1	1.98	0.64
1:A:216:ASN:HB2	2:A:1111:ACT:CH3	2.30	0.62
1:A:216:ASN:ND2	2:A:1111:ACT:H1	1.99	0.61
1:A:251:LYS:NZ	2:A:1109:ACT:H1	2.15	0.61
1:B:32:ARG:CD	3:B:1517:EDO:C1	2.53	0.61
1:A:216:ASN:HB2	2:A:1111:ACT:H3	1.83	0.59
3:A:1113:EDO:H12	8:A:1210:HOH:O	2.07	0.55
2:A:1111:ACT:H2	8:A:1297:HOH:O	2.08	0.54
1:B:84:HIS:HD2	8:B:1698:HOH:O	1.91	0.52
1:B:357:GLN:NE2	8:B:1601:HOH:O	2.41	0.52
1:A:305:TYR:OH	1:A:330:ILE:HD11	2.10	0.52
1:A:184:MET:HB3	2:A:1109:ACT:H2	1.93	0.51
1:B:85:ALA:HB1	1:B:94:LEU:HG	1.92	0.51
1:A:176:TYR:CG	5:A:1108:BME:H21	2.47	0.50
1:A:77:LEU:HD11	1:A:274:LYS:HD3	1.93	0.50
1:B:305:TYR:OH	1:B:330:ILE:HD11	2.12	0.49
5:A:1107:BME:S2	8:A:1373:HOH:O	2.60	0.49
3:A:1115:EDO:H12	8:A:1293:HOH:O	2.14	0.46
1:B:68:ALA:HA	3:B:1516:EDO:H12	1.98	0.44
1:A:63:VAL:HG21	3:A:1120:EDO:H12	2.00	0.43
1:A:307[A]:ASN:HA	4:A:1105:NAD:H2A	2.01	0.43
1:A:216:ASN:ND2	2:A:1111:ACT:CH3	2.68	0.43
1:A:327:TRP:CE2	1:B:164:ASN:HB3	2.54	0.42
1:B:324:ALA:HB1	1:B:329:LYS:HB2	2.02	0.42
1:A:298:ASN:OD1	1:B:159:ARG:NH2	2.48	0.41
1:B:206:MET:O	1:B:210:LEU:HG	2.20	0.41
1:B:42:TYR:O	1:B:46[B]:LEU:CD1	2.66	0.41
1:A:185:PRO:O	1:A:189:GLN:HG3	2.21	0.40
1:A:63:VAL:HG11	3:A:1120:EDO:H21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/369 (91%)	333 (99%)	3 (1%)	0	100	100
1	B	344/369 (93%)	338 (98%)	6 (2%)	0	100	100
All	All	680/738 (92%)	671 (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	287/309 (93%)	285 (99%)	2 (1%)	84	76
1	B	292/309 (94%)	290 (99%)	2 (1%)	84	76
All	All	579/618 (94%)	575 (99%)	4 (1%)	84	76

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

Mol	Chain	Res	Type
1	A	91	ARG
1	A	359	MET
1	B	91	ARG
1	B	357	GLN

Some 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 ⓘ

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	1.22	0	1,6,8	0.15	0
1	CSS	A	177	1	4,6,7	0.47	0	1,6,8	1.03	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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

40 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	$\# Z > 2$
3	EDO	A	1116	-	3,3,3	0.55	0	2,2,2	0.18	0
5	BME	B	1511	-	3,3,3	0.21	0	1,2,2	0.10	0
5	BME	A	1107	-	3,3,3	0.23	0	1,2,2	1.53	0
3	EDO	A	1114	-	3,3,3	0.14	0	2,2,2	0.65	0
4	NAD	A	1105	-	42,48,48	1.19	4 (9%)	50,73,73	1.78	12 (24%)
3	EDO	A	1119	-	3,3,3	0.41	0	2,2,2	0.13	0
3	EDO	A	1117	-	3,3,3	0.33	0	2,2,2	0.07	0
5	BME	A	1108	-	3,3,3	0.25	0	1,2,2	1.63	0
4	NAD	B	1510	-	42,48,48	1.03	2 (4%)	50,73,73	0.90	2 (4%)
2	ACT	B	1514	-	1,3,3	3.54	1 (100%)	0,3,3	0.00	-
3	EDO	A	1115	-	3,3,3	0.77	0	2,2,2	0.41	0
6	FMT	A	1122	-	0,2,2	0.00	-	0,1,1	0.00	-
3	EDO	B	1515	-	3,3,3	0.36	0	2,2,2	0.27	0
3	EDO	B	1507	-	3,3,3	0.41	0	2,2,2	0.57	0
3	EDO	A	1113	-	3,3,3	0.38	0	2,2,2	0.35	0
2	ACT	B	1512	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
2	ACT	A	1109	-	1,3,3	0.52	0	0,3,3	0.00	-
2	ACT	A	1104	-	1,3,3	6.17	1 (100%)	0,3,3	0.00	-
5	BME	A	1106	-	3,3,3	0.22	0	1,2,2	0.05	0
3	EDO	B	1504	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	A	1120	-	3,3,3	0.61	0	2,2,2	0.19	0
3	EDO	A	1121	-	3,3,3	0.59	0	2,2,2	0.36	0
2	ACT	B	1506	-	1,3,3	7.22	1 (100%)	0,3,3	0.00	-
7	MRD	B	1509	-	7,7,7	0.62	0	9,10,10	0.95	1 (11%)
2	ACT	B	1505	-	1,3,3	8.81	1 (100%)	0,3,3	0.00	-
3	EDO	A	1118	-	3,3,3	0.79	0	2,2,2	0.35	0
2	ACT	A	1110	-	1,3,3	4.79	1 (100%)	0,3,3	0.00	-
3	EDO	B	1516	-	3,3,3	0.36	0	2,2,2	0.03	0
3	EDO	B	1517	-	3,3,3	0.22	0	2,2,2	0.31	0
3	EDO	B	1508	-	3,3,3	0.42	0	2,2,2	0.35	0
2	ACT	A	1103	-	1,3,3	6.95	1 (100%)	0,3,3	0.00	-
2	ACT	A	1101	-	1,3,3	7.75	1 (100%)	0,3,3	0.00	-
3	EDO	A	1102	-	3,3,3	0.57	0	2,2,2	0.24	0
2	ACT	A	1112	-	1,3,3	2.21	1 (100%)	0,3,3	0.00	-
2	ACT	B	1503	-	1,3,3	8.40	1 (100%)	0,3,3	0.00	-
3	EDO	B	1518	-	3,3,3	0.63	0	2,2,2	0.40	0
2	ACT	A	1111	-	1,3,3	0.40	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	B	1502	-	1,3,3	7.66	1 (100%)	0,3,3	0.00	-
3	EDO	B	1501	-	3,3,3	0.28	0	2,2,2	0.52	0
2	ACT	B	1513	-	1,3,3	2.35	1 (100%)	0,3,3	0.00	-

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
3	EDO	A	1116	-	-	1/1/1/1	-
5	BME	B	1511	-	-	0/1/1/1	-
5	BME	A	1107	-	-	1/1/1/1	-
3	EDO	A	1114	-	-	1/1/1/1	-
4	NAD	A	1105	-	-	5/26/62/62	0/5/5/5
3	EDO	A	1119	-	-	1/1/1/1	-
3	EDO	A	1117	-	-	0/1/1/1	-
5	BME	A	1108	-	-	1/1/1/1	-
3	EDO	B	1508	-	-	0/1/1/1	-
3	EDO	A	1115	-	-	0/1/1/1	-
4	NAD	B	1510	-	-	4/26/62/62	0/5/5/5
3	EDO	B	1507	-	-	1/1/1/1	-
3	EDO	A	1113	-	-	0/1/1/1	-
3	EDO	B	1501	-	-	1/1/1/1	-
5	BME	A	1106	-	-	0/1/1/1	-
3	EDO	B	1504	-	-	0/1/1/1	-
3	EDO	A	1120	-	-	1/1/1/1	-
3	EDO	A	1121	-	-	1/1/1/1	-
7	MRD	B	1509	-	-	0/5/5/5	-
3	EDO	A	1118	-	-	1/1/1/1	-
3	EDO	B	1516	-	-	1/1/1/1	-
3	EDO	B	1517	-	-	1/1/1/1	-
3	EDO	A	1102	-	-	1/1/1/1	-
3	EDO	B	1518	-	-	1/1/1/1	-
3	EDO	B	1515	-	-	0/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1505	ACT	CH3-C	8.81	1.60	1.48
2	B	1503	ACT	CH3-C	8.40	1.59	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ACT	CH3-C	7.75	1.58	1.48
2	B	1502	ACT	CH3-C	7.66	1.58	1.48
2	B	1506	ACT	CH3-C	7.22	1.57	1.48
2	A	1103	ACT	CH3-C	6.95	1.57	1.48
2	A	1104	ACT	CH3-C	6.17	1.56	1.48
2	A	1110	ACT	CH3-C	4.79	1.54	1.48
2	B	1514	ACT	CH3-C	3.54	1.53	1.48
4	A	1105	NAD	C7N-N7N	-2.63	1.28	1.33
4	A	1105	NAD	PA-O2A	-2.52	1.43	1.55
4	B	1510	NAD	C8A-N7A	-2.49	1.30	1.34
4	A	1105	NAD	O2D-C2D	2.42	1.48	1.43
2	B	1513	ACT	CH3-C	2.35	1.51	1.48
2	B	1512	ACT	CH3-C	2.26	1.51	1.48
2	A	1112	ACT	CH3-C	2.21	1.51	1.48
4	A	1105	NAD	C3D-C4D	2.14	1.58	1.53
4	B	1510	NAD	PN-O2N	-2.00	1.45	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1105	NAD	O4D-C1D-C2D	-5.34	99.12	106.93
4	A	1105	NAD	C3D-C2D-C1D	4.51	107.76	100.98
4	A	1105	NAD	C5N-C4N-C3N	-3.74	115.92	120.34
4	A	1105	NAD	O7N-C7N-C3N	3.20	123.46	119.63
4	A	1105	NAD	O2A-PA-O1A	3.18	127.98	112.24
4	A	1105	NAD	C3N-C7N-N7N	-3.18	113.94	117.75
4	B	1510	NAD	O4D-C1D-C2D	-2.85	102.76	106.93
4	A	1105	NAD	O2B-C2B-C3B	-2.67	103.19	111.82
4	A	1105	NAD	C2N-C3N-C4N	2.62	121.23	118.26
4	B	1510	NAD	C5A-C6A-N6A	2.55	124.23	120.35
4	A	1105	NAD	C6N-C5N-C4N	2.36	122.87	119.44
7	B	1509	MRD	CM-C2-C1	-2.35	105.67	110.57
4	A	1105	NAD	O4B-C4B-C3B	-2.19	100.79	105.11
4	A	1105	NAD	N6A-C6A-N1A	2.07	122.88	118.57
4	A	1105	NAD	N3A-C2A-N1A	-2.01	125.54	128.68

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1105	NAD	C5D-O5D-PN-O2N
5	A	1108	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
4	B	1510	NAD	PA-O3-PN-O5D
4	B	1510	NAD	C5D-O5D-PN-O2N
3	A	1102	EDO	O1-C1-C2-O2
3	A	1120	EDO	O1-C1-C2-O2
3	B	1517	EDO	O1-C1-C2-O2
3	A	1114	EDO	O1-C1-C2-O2
3	A	1119	EDO	O1-C1-C2-O2
3	B	1516	EDO	O1-C1-C2-O2
5	A	1107	BME	O1-C1-C2-S2
4	A	1105	NAD	PA-O3-PN-O5D
4	A	1105	NAD	C5D-O5D-PN-O3
4	B	1510	NAD	C5D-O5D-PN-O3
4	A	1105	NAD	C5D-O5D-PN-O1N
4	B	1510	NAD	C5D-O5D-PN-O1N
3	A	1118	EDO	O1-C1-C2-O2
3	A	1121	EDO	O1-C1-C2-O2
3	B	1501	EDO	O1-C1-C2-O2
3	B	1518	EDO	O1-C1-C2-O2
3	A	1116	EDO	O1-C1-C2-O2
3	B	1507	EDO	O1-C1-C2-O2
4	A	1105	NAD	PA-O3-PN-O1N

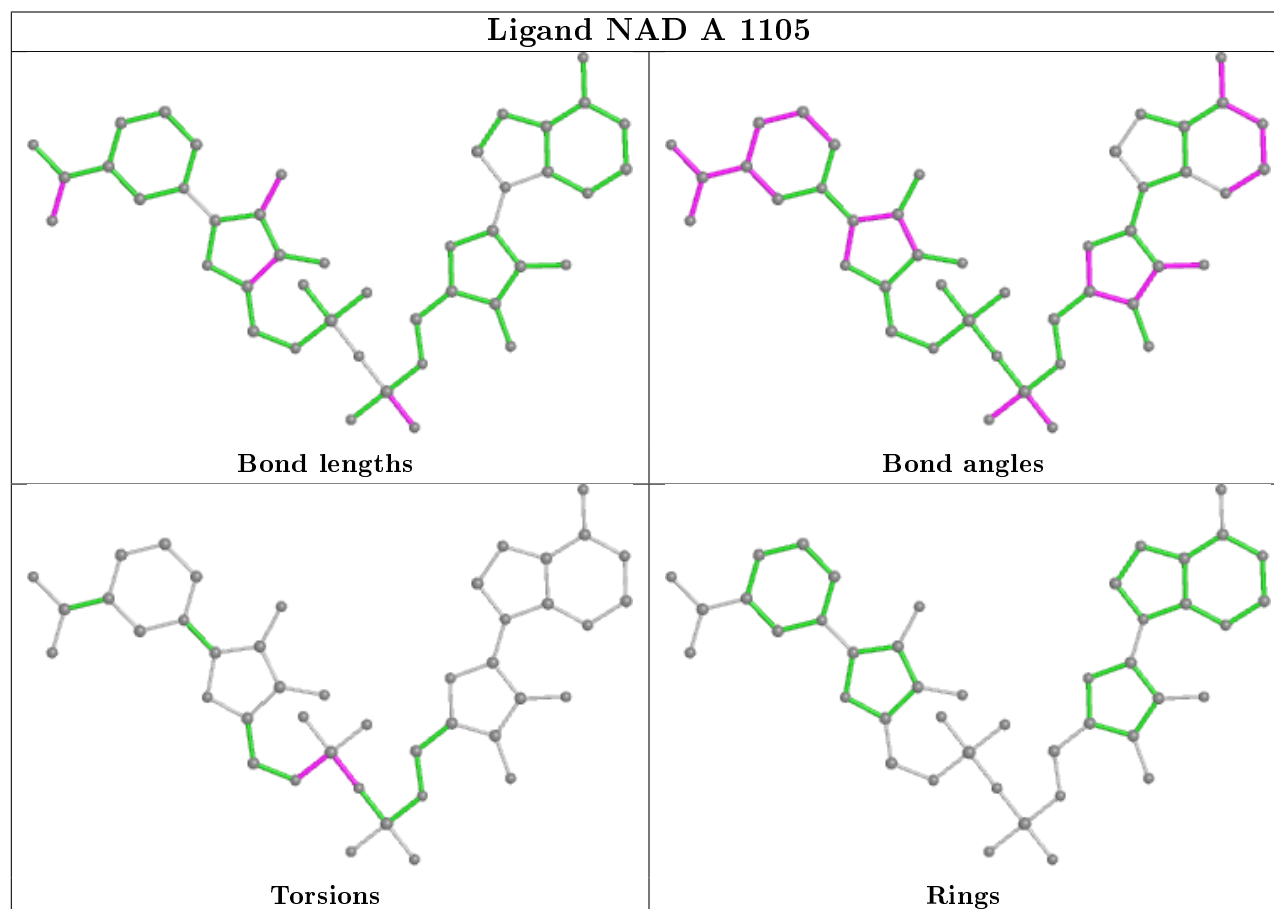
There are no ring outliers.

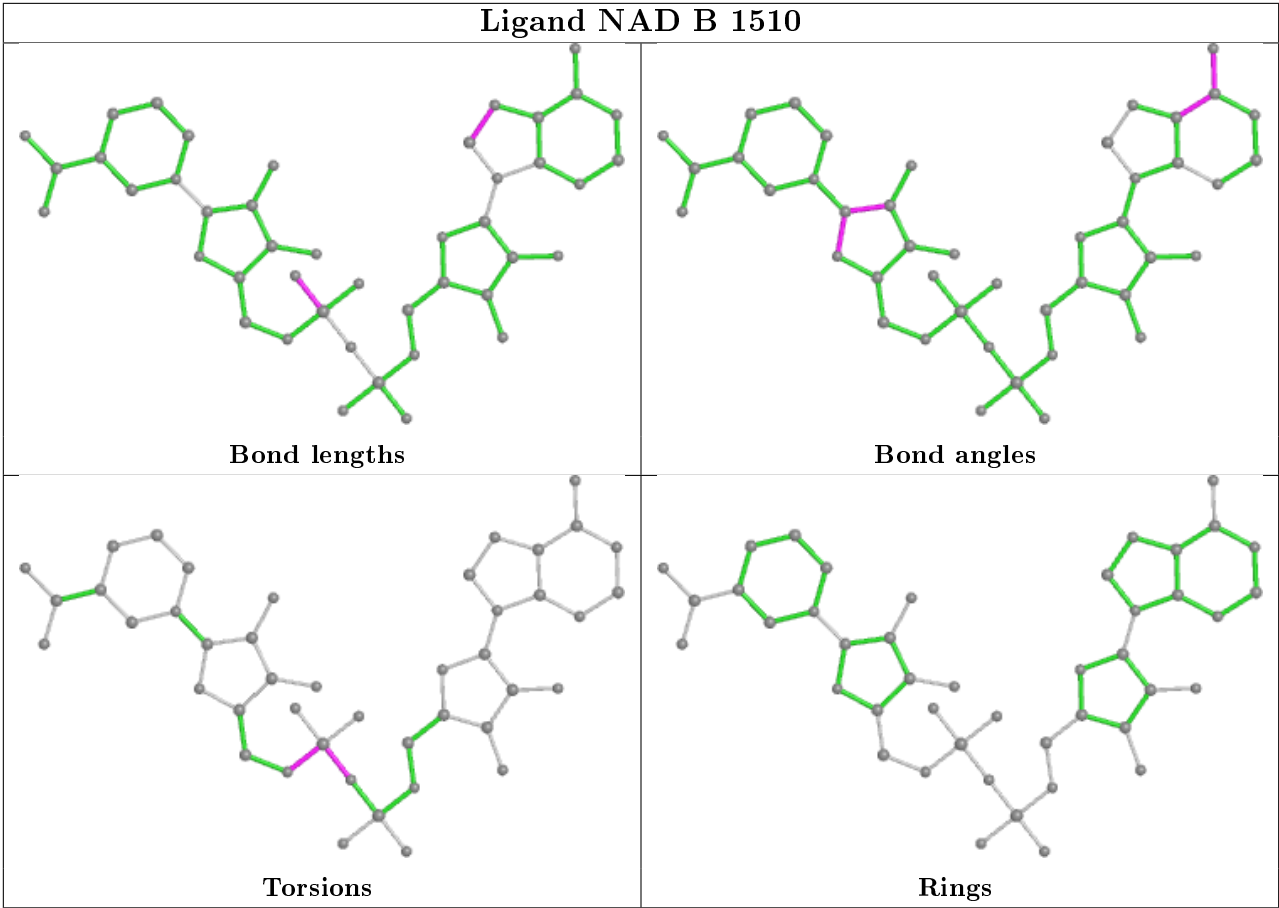
11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1107	BME	1	0
4	A	1105	NAD	1	0
3	A	1119	EDO	1	0
5	A	1108	BME	1	0
3	A	1115	EDO	1	0
3	A	1113	EDO	2	0
2	A	1109	ACT	2	0
3	A	1120	EDO	2	0
3	B	1516	EDO	1	0
3	B	1517	EDO	7	0
2	A	1111	ACT	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	362:PHE	C	363:MET	N	0.95

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	329/369 (89%)	-0.03	19 (5%) 23 24	23, 31, 71, 112	0
1	B	336/369 (91%)	0.12	29 (8%) 10 11	22, 32, 70, 152	0
All	All	665/738 (90%)	0.05	48 (7%) 15 16	22, 32, 71, 152	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	7.1
1	A	77	LEU	6.4
1	B	85	ALA	5.6
1	B	370	HIS	4.7
1	B	91	ARG	4.7
1	B	28	SER	4.7
1	A	85	ALA	4.6
1	B	94	LEU	4.4
1	A	363	MET	4.4
1	A	86	ASP	4.0
1	B	77	LEU	3.8
1	B	90	SER	3.7
1	B	89	GLN	3.2
1	B	79	GLN	3.1
1	B	88	THR	3.1
1	B	86	ASP	3.1
1	A	76	PRO	3.0
1	A	84	HIS	3.0
1	B	82	ASP	3.0
1	B	286	VAL	2.9
1	B	93	PRO	2.9
1	B	84	HIS	2.9
1	A	362	PHE	2.8
1	A	341	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	285[A]	VAL	2.7
1	B	80	ASP	2.7
1	A	309	ALA	2.7
1	B	285	VAL	2.6
1	A	235	ALA	2.6
1	B	76	PRO	2.4
1	B	309	ALA	2.4
1	B	78	SER	2.4
1	A	91	ARG	2.4
1	A	312	PHE	2.3
1	B	312	PHE	2.3
1	B	235	ALA	2.2
1	A	332	VAL	2.2
1	A	94	LEU	2.2
1	A	283	GLY	2.2
1	B	83	GLN	2.2
1	A	234	PRO	2.2
1	B	160	GLU	2.2
1	B	192	MET	2.2
1	A	340	TYR	2.1
1	B	196	THR	2.0
1	B	158	LEU	2.0
1	B	308[A]	THR	2.0
1	B	87	LEU	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(\AA^2)	Q<0.9
1	CSS	B	177	7/8	0.97	0.10	37,54,86,103	0
1	CSS	A	177	7/8	0.98	0.05	31,40,64,77	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
3	EDO	B	1504	4/4	0.64	0.41	88,108,130,130	0
3	EDO	A	1114	4/4	0.68	0.17	71,86,96,96	0
3	EDO	B	1517	4/4	0.73	0.51	73,101,119,130	0
2	ACT	B	1505	4/4	0.79	0.15	68,80,82,82	0
2	ACT	B	1513	4/4	0.79	0.30	92,102,126,126	0
3	EDO	A	1102	4/4	0.80	0.26	60,73,87,105	0
2	ACT	B	1502	4/4	0.80	0.37	89,93,107,107	0
5	BME	A	1108	4/4	0.80	0.14	56,77,101,102	0
2	ACT	A	1103	4/4	0.81	0.21	67,73,80,80	0
2	ACT	B	1503	4/4	0.81	0.30	75,78,90,90	0
2	ACT	A	1101	4/4	0.83	0.23	63,75,77,83	0
2	ACT	A	1111	4/4	0.83	0.17	67,74,94,94	0
3	EDO	B	1516	4/4	0.84	0.32	64,89,107,107	0
2	ACT	B	1514	4/4	0.84	0.21	73,80,88,88	0
2	ACT	A	1110	4/4	0.84	0.17	63,66,75,75	0
3	EDO	B	1507	4/4	0.85	0.35	65,79,84,89	10
3	EDO	A	1121	4/4	0.86	0.13	44,59,80,85	0
5	BME	B	1511	4/4	0.86	0.24	46,61,73,75	10
3	EDO	A	1119	4/4	0.86	0.35	41,76,91,91	10
3	EDO	A	1113	4/4	0.87	0.22	37,46,75,91	10
3	EDO	B	1515	4/4	0.87	0.20	76,91,95,102	0
3	EDO	B	1508	4/4	0.88	0.22	74,89,94,98	0
5	BME	A	1106	4/4	0.88	0.10	45,78,112,121	0
5	BME	A	1107	4/4	0.88	0.10	77,92,112,134	0
3	EDO	B	1501	4/4	0.89	0.15	44,57,59,69	10
6	FMT	A	1122	3/3	0.90	0.20	79,80,80,96	0
2	ACT	A	1104	4/4	0.91	0.13	49,59,64,73	7
3	EDO	A	1117	4/4	0.91	0.09	63,97,112,124	0
3	EDO	A	1116	4/4	0.92	0.26	38,52,66,66	10
2	ACT	B	1512	4/4	0.92	0.16	52,62,78,85	0
3	EDO	A	1120	4/4	0.93	0.10	39,47,57,57	10
3	EDO	B	1518	4/4	0.94	0.08	33,52,64,64	0
2	ACT	B	1506	4/4	0.94	0.10	67,78,102,102	0
3	EDO	A	1118	4/4	0.94	0.18	46,82,98,98	0
2	ACT	A	1112	4/4	0.94	0.41	66,76,79,79	0
7	MRD	B	1509	8/8	0.94	0.11	38,54,71,71	0
2	ACT	A	1109	4/4	0.95	0.12	25,30,69,98	0

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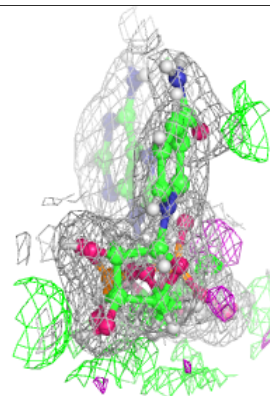
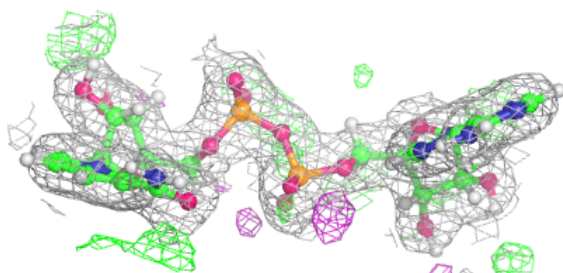
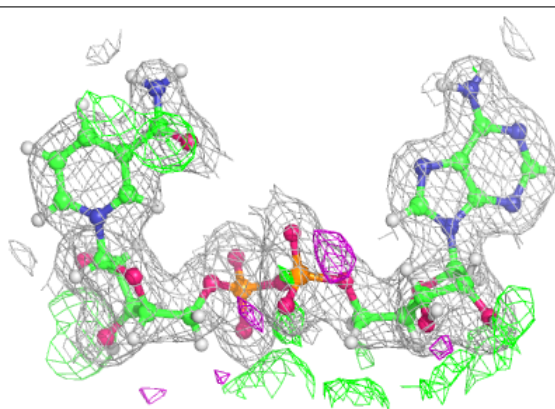
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAD	B	1510	44/44	0.97	0.13	22,30,42,44	0
3	EDO	A	1115	4/4	0.97	0.08	38,54,65,71	10
4	NAD	A	1105	44/44	0.98	0.16	19,26,40,43	0

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.

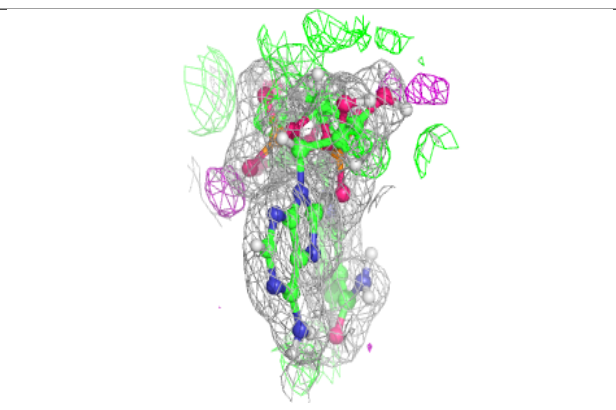
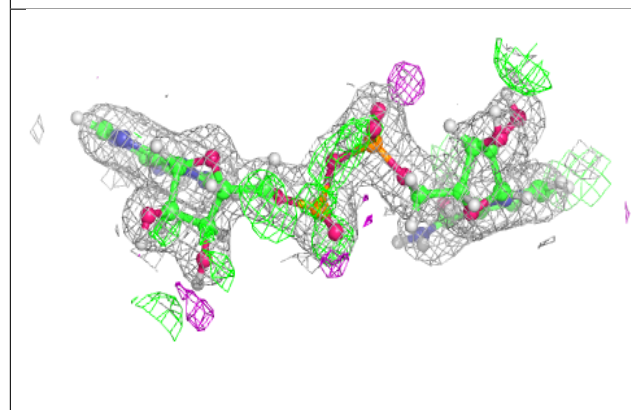
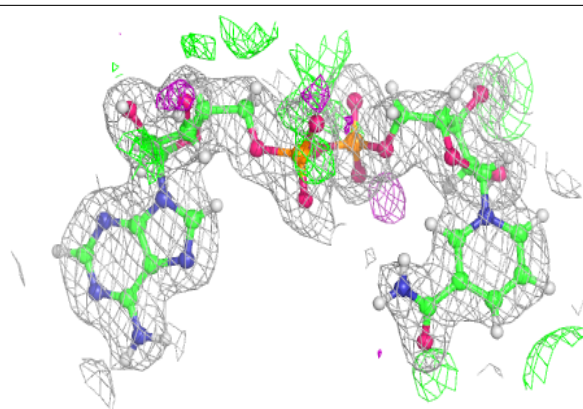
Electron density around NAD B 1510:

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 1105:

$2mF_o - DF_c$ (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.