



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:39 AM BST

PDB ID : 6ADE
Title : Crystal structure of phosphorylated mutant of glyceraldehyde 3-phosphate dehydrogenase from human placenta at 3.15Å resolution
Authors : Dilawari, R.; Singh, P.K.; Raje, M.; Sharma, S.; Singh, T.P.
Deposited on : 2018-07-31
Resolution : 3.15 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	:	2.13.1
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)	:	2.13.1

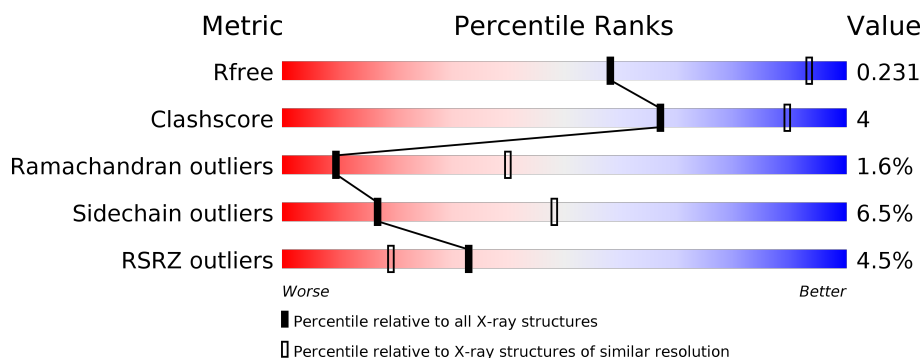
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	335	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	335	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	335	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7679 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.

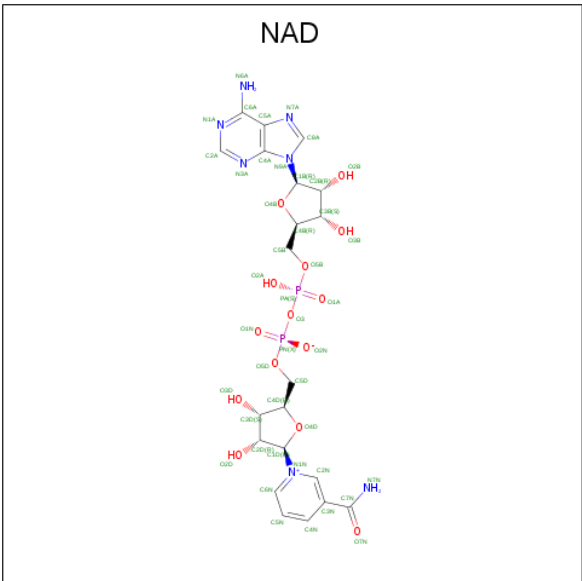
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	P	S	0	0	0
			2530	1596	437	483	2	12			
1	B	333	Total	C	N	O	P	S	0	0	0
			2530	1596	437	483	2	12			
1	C	333	Total	C	N	O	P	S	0	0	0
			2530	1596	437	483	2	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LEU	LYS	engineered mutation	UNP P04406
B	271	LEU	LYS	engineered mutation	UNP P04406
C	271	LEU	LYS	engineered mutation	UNP P04406

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

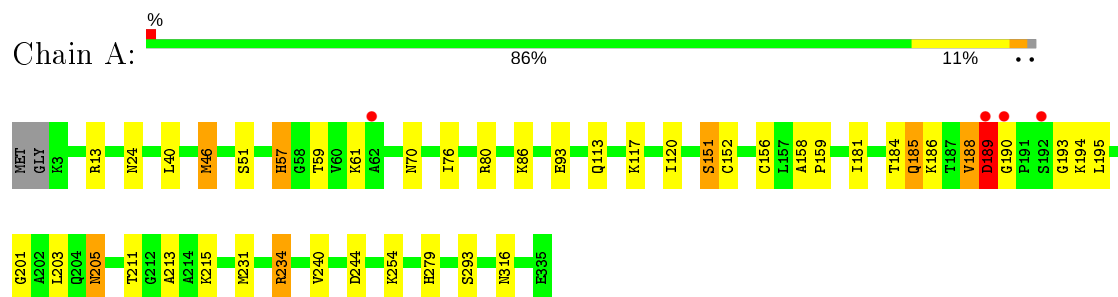
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	17	Total	O	0	0
			17	17		
3	C	7	Total	O	0	0
			7	7		

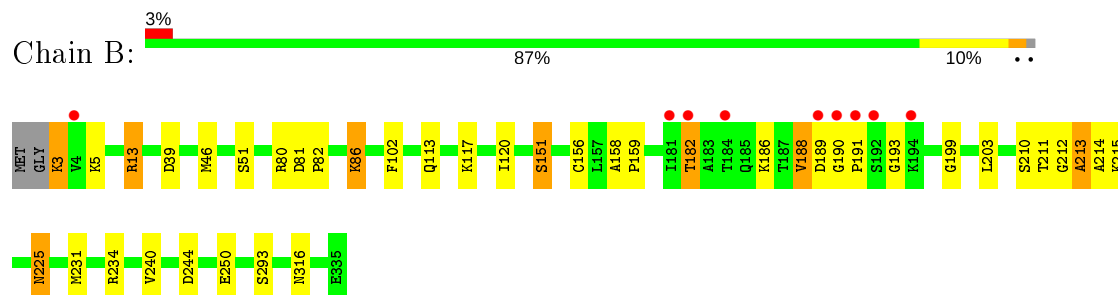
3 Residue-property plots [i](#)

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.

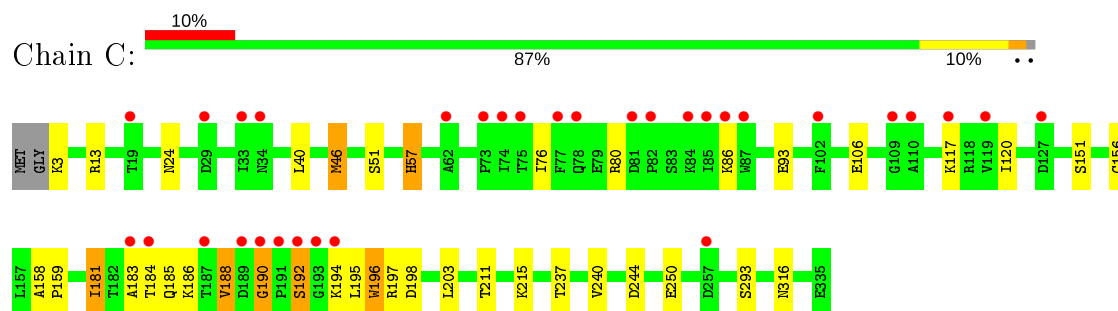
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.78Å 131.68Å 220.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.39 – 3.15 45.39 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.39-3.15) 99.9 (45.39-3.15)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.194 , 0.239 0.198 , 0.231	Depositor DCC
R_{free} test set	1161 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: NAD, SEP

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	0.45	0/2558	0.65	0/3459
1	B	0.43	0/2558	0.65	0/3459
1	C	0.42	0/2558	0.64	0/3459
All	All	0.43	0/7674	0.65	0/10377

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	2
1	B	0	2
1	C	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	234	ARG	Sidechain
1	B	13	ARG	Sidechain
1	B	182	THR	Peptide
1	C	13	ARG	Sidechain
1	C	195	LEU	Peptide
1	C	80	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2530	0	2520	23	0
1	B	2530	0	2520	23	0
1	C	2530	0	2520	15	0
2	A	44	0	26	4	0
3	A	21	0	0	0	0
3	B	17	0	0	1	0
3	C	7	0	0	0	0
All	All	7679	0	7586	60	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 (60) 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:186:LYS:HD3	1:B:190:GLY:HA2	1.53	0.89
1:B:189:ASP:OD2	3:B:401:HOH:O	1.92	0.86
1:A:181:ILE:HG22	1:A:185:GLN:NE2	1.98	0.78
1:A:181:ILE:HG22	1:A:185:GLN:HE22	1.47	0.77
1:A:113:GLN:HA	1:B:113:GLN:HA	1.67	0.77
1:A:24:ASN:ND2	1:A:57:HIS:NE2	2.34	0.73
1:B:186:LYS:CD	1:B:190:GLY:HA2	2.20	0.71
1:A:201:GLY:O	1:A:205:ASN:ND2	2.24	0.69
1:B:212:GLY:O	1:B:214:ALA:N	2.25	0.69
1:C:183:ALA:O	1:C:185:GLN:N	2.27	0.67
1:A:151:SEP:O1P	1:A:213:ALA:HB2	1.94	0.66
1:C:186:LYS:HD2	1:C:190:GLY:HA3	1.77	0.65
1:C:186:LYS:CD	1:C:190:GLY:HA3	2.29	0.63
1:C:181:ILE:HD13	1:C:237:THR:O	2.00	0.61
1:A:234:ARG:HH21	1:A:234:ARG:HG3	1.66	0.58
1:C:196:TRP:O	1:C:198:ASP:N	2.36	0.58
1:A:24:ASN:OD1	1:A:57:HIS:CD2	2.58	0.56
1:B:186:LYS:HD3	1:B:190:GLY:CA	2.32	0.56
1:B:190:GLY:HA3	1:B:199:GLY:O	2.06	0.56
1:C:186:LYS:HG3	1:C:190:GLY:HA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:CYS:HA	1:B:293:SER:HB2	1.89	0.54
1:A:46:MET:CE	1:A:46:MET:HA	2.39	0.53
1:C:186:LYS:CG	1:C:190:GLY:HA3	2.39	0.53
1:C:46:MET:HA	1:C:46:MET:CE	2.38	0.53
1:A:156:CYS:HA	1:A:293:SER:HB2	1.91	0.53
1:B:186:LYS:NZ	1:B:191:PRO:O	2.38	0.52
1:C:156:CYS:HA	1:C:293:SER:HB2	1.92	0.52
1:B:182:THR:OG1	1:B:234:ARG:NH1	2.39	0.51
1:B:186:LYS:HE2	1:B:190:GLY:HA2	1.92	0.51
1:A:186:LYS:HB3	1:A:189:ASP:OD1	2.12	0.50
1:C:186:LYS:HD2	1:C:190:GLY:CA	2.42	0.50
1:A:152:CYS:HB3	2:A:401:NAD:H5N	1.92	0.50
1:B:186:LYS:CE	1:B:190:GLY:HA2	2.43	0.48
1:B:211:THR:O	1:B:211:THR:HG23	2.14	0.47
1:C:158:ALA:HB3	1:C:159:PRO:HD3	1.97	0.47
1:A:158:ALA:HB3	1:A:159:PRO:HD3	1.97	0.46
1:B:158:ALA:HB3	1:B:159:PRO:HD3	1.97	0.46
1:B:151:SEP:O2P	1:B:213:ALA:HB2	2.17	0.45
1:C:24:ASN:OD1	1:C:57:HIS:HD2	2.00	0.45
1:A:40:LEU:HD13	1:A:76:ILE:HG13	2.00	0.44
1:A:46:MET:HA	1:A:46:MET:HE2	1.99	0.44
1:A:152:CYS:HB3	2:A:401:NAD:C5N	2.48	0.44
1:A:211:THR:HG23	1:A:211:THR:O	2.18	0.43
1:B:82:PRO:HG3	1:B:102:PHE:CE2	2.54	0.43
1:A:152:CYS:HB3	2:A:401:NAD:H4N	2.01	0.43
1:C:211:THR:HG23	1:C:211:THR:O	2.19	0.42
1:A:211:THR:HG22	1:A:231:MET:HA	2.01	0.42
1:B:86:LYS:CD	1:B:86:LYS:H	2.32	0.42
1:B:211:THR:HG22	1:B:231:MET:HA	2.01	0.42
1:B:3:LYS:HE3	1:B:3:LYS:HA	2.01	0.42
1:A:59:THR:CG2	1:A:70:ASN:HA	2.50	0.41
1:B:120:ILE:N	1:B:120:ILE:HD12	2.35	0.41
1:A:205:ASN:N	1:A:205:ASN:ND2	2.67	0.41
1:B:186:LYS:HE2	1:B:191:PRO:HD2	2.02	0.41
1:A:152:CYS:HB3	2:A:401:NAD:C4N	2.51	0.41
1:B:225:ASN:HD22	1:B:225:ASN:C	2.23	0.40
1:B:81:ASP:HA	1:B:82:PRO:HD3	1.98	0.40
1:C:120:ILE:HD12	1:C:120:ILE:N	2.37	0.40
1:A:120:ILE:N	1:A:120:ILE:HD12	2.37	0.40
1:C:40:LEU:HD13	1:C:76:ILE:HG13	2.03	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	329/335 (98%)	310 (94%)	14 (4%)	5 (2%)	10	41
1	B	329/335 (98%)	308 (94%)	17 (5%)	4 (1%)	13	46
1	C	329/335 (98%)	302 (92%)	20 (6%)	7 (2%)	7	33
All	All	987/1005 (98%)	920 (93%)	51 (5%)	16 (2%)	9	40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	ASP
1	B	188	VAL
1	B	193	GLY
1	B	213	ALA
1	C	184	THR
1	A	188	VAL
1	A	193	GLY
1	C	188	VAL
1	C	197	ARG
1	A	240	VAL
1	B	240	VAL
1	C	240	VAL
1	C	192	SER
1	C	196	TRP
1	A	190	GLY
1	C	190	GLY

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	268/269 (100%)	248 (92%)	20 (8%)	13	42
1	B	268/269 (100%)	252 (94%)	16 (6%)	19	51
1	C	268/269 (100%)	252 (94%)	16 (6%)	19	51
All	All	804/807 (100%)	752 (94%)	52 (6%)	17	48

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	57	HIS
1	A	61	LYS
1	A	80	ARG
1	A	86	LYS
1	A	93	GLU
1	A	117	LYS
1	A	184	THR
1	A	185	GLN
1	A	188	VAL
1	A	189	ASP
1	A	194	LYS
1	A	195	LEU
1	A	203	LEU
1	A	205	ASN
1	A	215	LYS
1	A	244	ASP
1	A	254	LYS
1	A	279	HIS
1	A	316	ASN
1	B	3	LYS
1	B	5	LYS
1	B	13	ARG
1	B	39	ASP
1	B	46	MET
1	B	80	ARG
1	B	86	LYS
1	B	117	LYS
1	B	188	VAL
1	B	203	LEU
1	B	210	SER
1	B	215	LYS

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Mol	Chain	Res	Type
1	B	225	ASN
1	B	244	ASP
1	B	250	GLU
1	B	316	ASN
1	C	3	LYS
1	C	46	MET
1	C	57	HIS
1	C	86	LYS
1	C	93	GLU
1	C	106	GLU
1	C	117	LYS
1	C	181	ILE
1	C	188	VAL
1	C	192	SER
1	C	194	LYS
1	C	203	LEU
1	C	215	LYS
1	C	244	ASP
1	C	250	GLU
1	C	316	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	225	ASN
1	C	142	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 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	SEP	B	51	1	8,9,10	1.27	1 (12%)	8,12,14	3.71	3 (37%)
1	SEP	C	151	1	8,9,10	1.73	2 (25%)	8,12,14	6.42	3 (37%)
1	SEP	B	151	1	8,9,10	1.86	2 (25%)	8,12,14	5.59	2 (25%)
1	SEP	A	51	1	8,9,10	1.25	1 (12%)	8,12,14	5.14	4 (50%)
1	SEP	C	51	1	8,9,10	1.34	2 (25%)	8,12,14	4.23	2 (25%)
1	SEP	A	151	1	8,9,10	2.17	2 (25%)	8,12,14	6.92	3 (37%)

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	SEP	B	51	1	-	5/5/8/10	-
1	SEP	C	151	1	-	2/5/8/10	-
1	SEP	B	151	1	-	4/5/8/10	-
1	SEP	A	51	1	-	4/5/8/10	-
1	SEP	C	51	1	-	5/5/8/10	-
1	SEP	A	151	1	-	1/5/8/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	SEP	P-OG	4.85	1.75	1.60
1	C	151	SEP	P-OG	3.57	1.71	1.60
1	B	151	SEP	P-OG	3.44	1.71	1.60
1	A	151	SEP	CB-CA	3.02	1.61	1.52
1	A	51	SEP	P-OG	2.97	1.69	1.60
1	B	151	SEP	CB-CA	2.92	1.60	1.52
1	C	151	SEP	CB-CA	2.72	1.60	1.52
1	B	51	SEP	P-OG	2.71	1.68	1.60
1	C	51	SEP	P-OG	2.63	1.68	1.60
1	C	51	SEP	CB-CA	2.16	1.58	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	SEP	OG-CB-CA	18.23	125.88	108.14
1	C	151	SEP	OG-CB-CA	16.77	124.47	108.14
1	B	151	SEP	OG-CB-CA	14.62	122.37	108.14
1	C	51	SEP	OG-CB-CA	11.33	119.17	108.14
1	A	51	SEP	P-OG-CB	10.09	146.09	118.30
1	A	51	SEP	OG-CB-CA	9.36	117.26	108.14
1	B	51	SEP	OG-CB-CA	8.89	116.80	108.14
1	A	151	SEP	P-OG-CB	6.05	134.97	118.30
1	C	151	SEP	P-OG-CB	5.99	134.80	118.30
1	B	151	SEP	P-OG-CB	5.58	133.66	118.30
1	B	51	SEP	P-OG-CB	4.68	131.17	118.30
1	A	151	SEP	O3P-P-OG	3.63	116.39	106.73
1	C	51	SEP	P-OG-CB	3.54	128.04	118.30
1	A	51	SEP	O3P-P-OG	-3.19	98.24	106.73
1	C	151	SEP	O3P-P-O2P	2.54	117.35	107.64
1	A	51	SEP	OG-P-O1P	2.52	113.54	106.47
1	B	51	SEP	O3P-P-O2P	2.09	115.63	107.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	51	SEP	N-CA-CB-OG
1	B	51	SEP	CA-CB-OG-P
1	B	51	SEP	CB-OG-P-O1P
1	B	51	SEP	CB-OG-P-O2P
1	B	51	SEP	CB-OG-P-O3P
1	C	151	SEP	N-CA-CB-OG
1	C	151	SEP	CB-OG-P-O3P
1	B	151	SEP	N-CA-CB-OG
1	B	151	SEP	CB-OG-P-O2P
1	B	151	SEP	CB-OG-P-O3P
1	A	51	SEP	N-CA-CB-OG
1	A	51	SEP	CB-OG-P-O2P
1	A	51	SEP	CB-OG-P-O3P
1	C	51	SEP	N-CA-CB-OG
1	C	51	SEP	CA-CB-OG-P
1	C	51	SEP	CB-OG-P-O3P
1	A	151	SEP	N-CA-CB-OG
1	B	151	SEP	CB-OG-P-O1P
1	C	51	SEP	CB-OG-P-O1P
1	C	51	SEP	CB-OG-P-O2P
1	A	51	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	151	SEP	1	0
1	A	151	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	NAD	A	401	-	42,48,48	1.17	3 (7%)	50,73,73	1.35	6 (12%)

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	NAD	A	401	-	-	14/26/62/62	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	O4D-C1D	3.88	1.46	1.41
2	A	401	NAD	C5A-C4A	2.88	1.48	1.40
2	A	401	NAD	C2A-N3A	2.86	1.36	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	O5D-C5D-C4D	3.45	120.86	108.99
2	A	401	NAD	C2D-C3D-C4D	3.45	109.34	102.64
2	A	401	NAD	C4A-C5A-N7A	-3.21	106.06	109.40
2	A	401	NAD	N3A-C2A-N1A	-3.01	123.98	128.68
2	A	401	NAD	C3D-C2D-C1D	2.16	104.23	100.98
2	A	401	NAD	C3N-C2N-N1N	2.08	122.46	120.43

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	C5B-O5B-PA-O2A
2	A	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O2N
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	C3D-C4D-C5D-O5D
2	A	401	NAD	PN-O3-PA-O5B
2	A	401	NAD	C5B-O5B-PA-O3
2	A	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	C2D-C1D-N1N-C6N

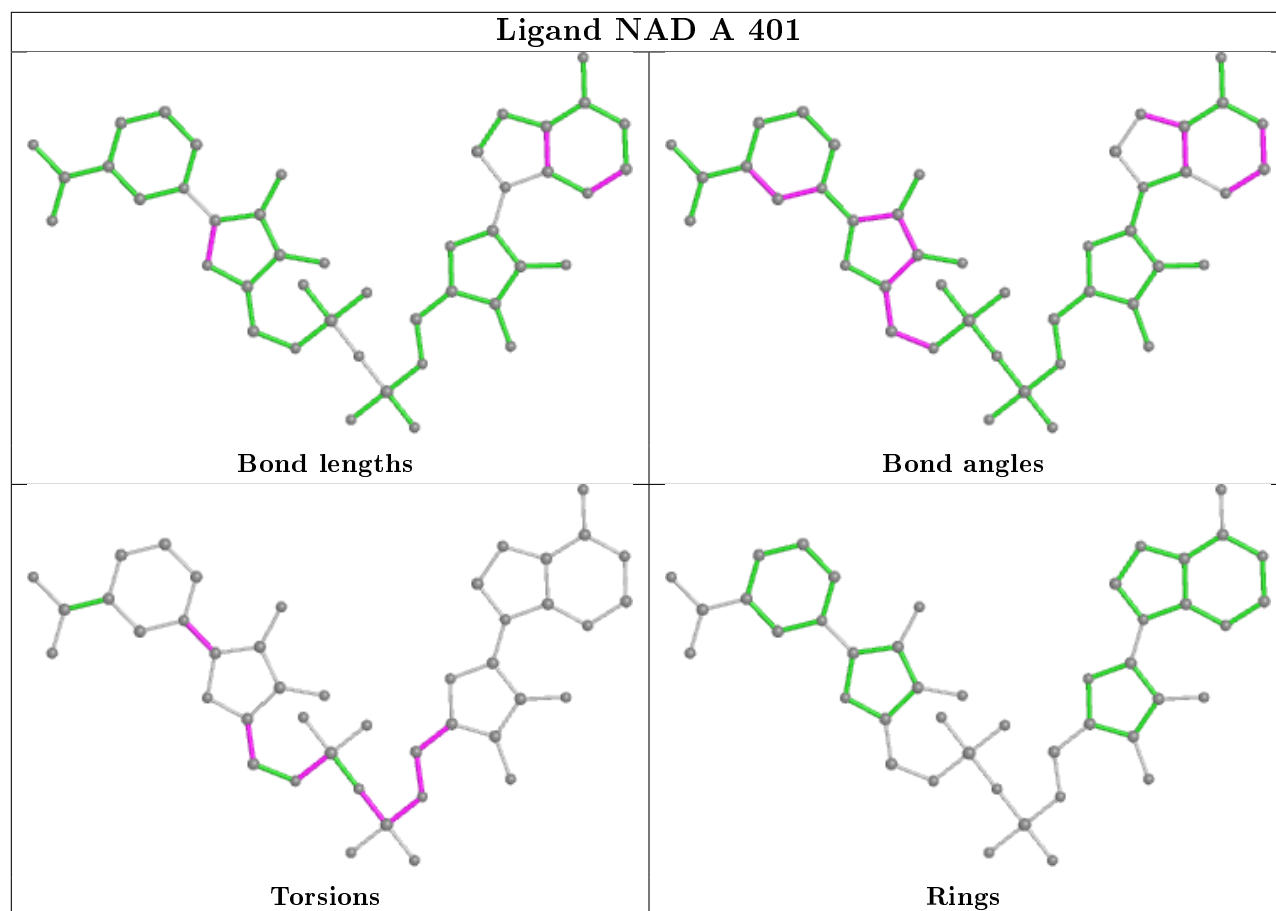
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	4	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	331/335 (98%)	-0.01	4 (1%) 79 68	33, 57, 91, 228	0
1	B	331/335 (98%)	0.32	9 (2%) 54 38	47, 68, 103, 198	0
1	C	331/335 (98%)	0.64	32 (9%) 7 4	45, 87, 132, 221	0
All	All	993/1005 (98%)	0.32	45 (4%) 33 19	33, 70, 122, 228	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	ASP	4.7
1	B	190	GLY	4.5
1	C	191	PRO	4.5
1	B	182	THR	4.2
1	C	190	GLY	4.0
1	A	189	ASP	3.5
1	C	192	SER	3.5
1	C	86	LYS	3.4
1	C	189	ASP	3.4
1	C	257	ASP	3.2
1	C	85	ILE	3.2
1	B	191	PRO	3.2
1	C	73	PRO	3.1
1	B	184	THR	3.0
1	C	82	PRO	3.0
1	C	193	GLY	2.9
1	B	194	LYS	2.8
1	C	194	LYS	2.6
1	C	34	ASN	2.6
1	C	62	ALA	2.4
1	C	33	ILE	2.4
1	C	109	GLY	2.4
1	C	117	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	29	ASP	2.4
1	C	187	THR	2.3
1	C	127	ASP	2.3
1	C	84	LYS	2.3
1	C	75	THR	2.3
1	C	77	PHE	2.3
1	C	119	VAL	2.2
1	C	110	ALA	2.1
1	C	81	ASP	2.1
1	A	192	SER	2.1
1	C	78	GLN	2.1
1	C	102	PHE	2.1
1	C	74	ILE	2.1
1	B	192	SER	2.1
1	A	62	ALA	2.1
1	B	4	VAL	2.1
1	C	87	TRP	2.1
1	C	183	ALA	2.0
1	C	184	THR	2.0
1	A	190	GLY	2.0
1	B	181	ILE	2.0
1	C	19	THR	2.0

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
1	SEP	C	151	10/11	0.86	0.19	62,88,108,109	0
1	SEP	B	151	10/11	0.86	0.25	56,72,99,106	0
1	SEP	A	151	10/11	0.92	0.20	45,64,87,88	0
1	SEP	C	51	10/11	0.96	0.21	64,72,75,75	0
1	SEP	A	51	10/11	0.96	0.22	45,53,60,65	0
1	SEP	B	51	10/11	0.97	0.24	47,61,70,76	0

6.3 Carbohydrates ⓘ

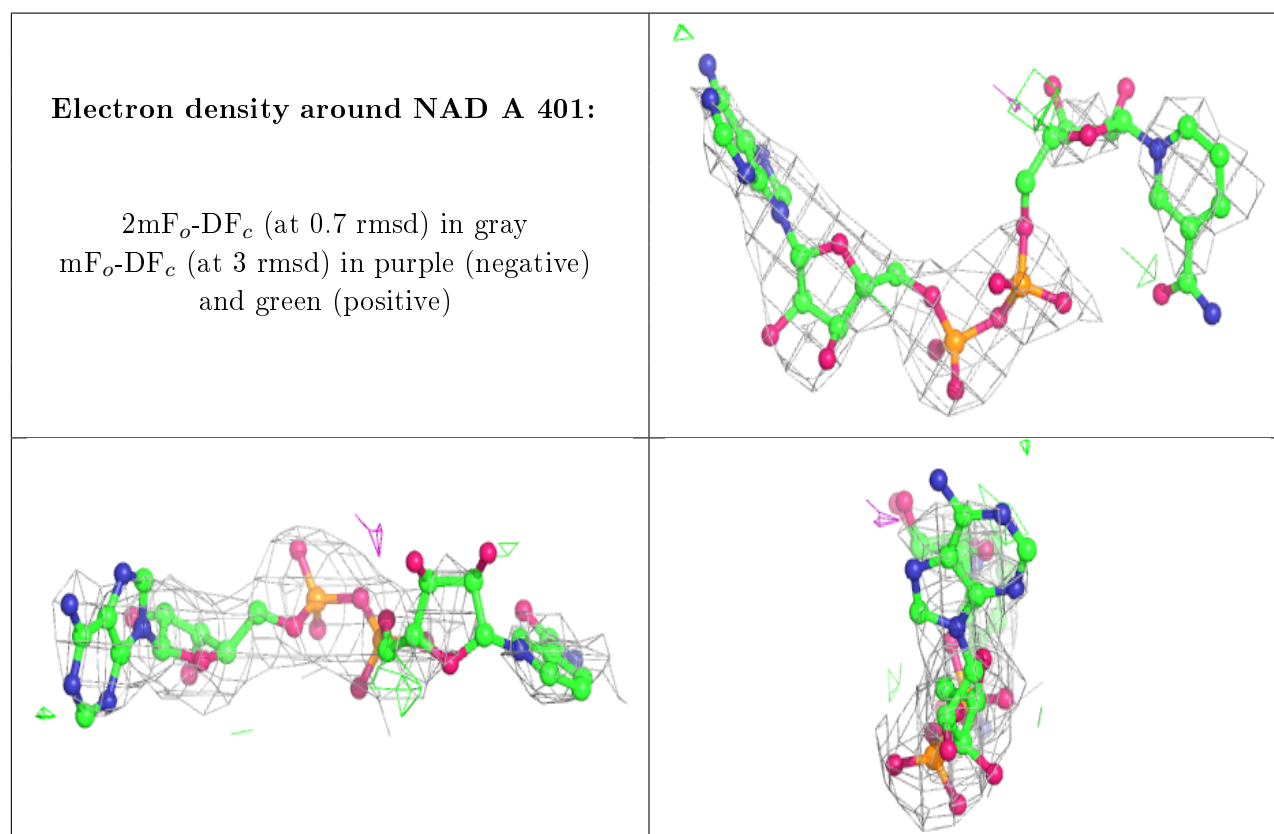
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	A	401	44/44	0.88	0.30	70,85,117,126	44

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.