



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:53 AM UTC

PDB ID : 7EOZ / pdb_00007eoz
Title : The structure of rice Defective Pollen Wall (DPW) in the complex with its cofactor NADP
Authors : Yan, L.M.; Wang, W.; Li, G.; Wang, J.
Deposited on : 2021-04-24
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

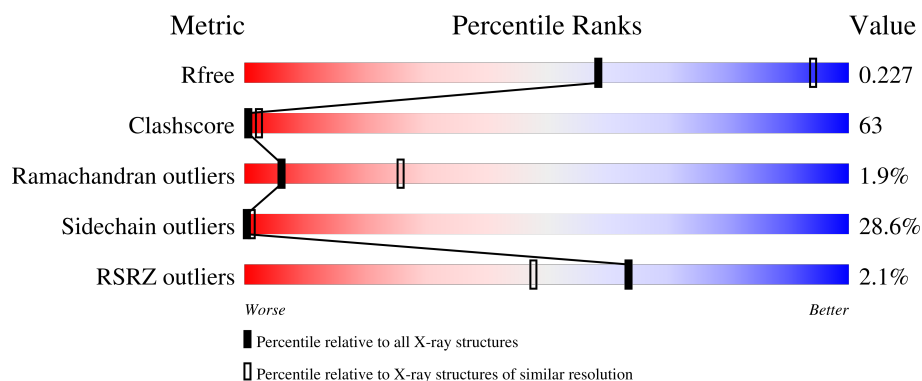
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	532	2% 29% 36% 22% 9%
1	B	532	% 27% 37% 20% 5% 11%

2 Entry composition [i](#)

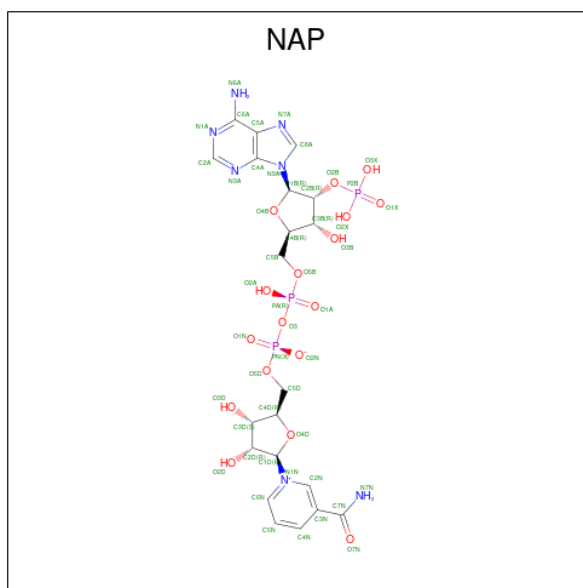
There are 3 unique types of molecules in this entry. The entry contains 7616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fatty acyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3753	2387	654	694	18			
1	B	473	Total	C	N	O	S	0	0	0
			3682	2344	639	681	18			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

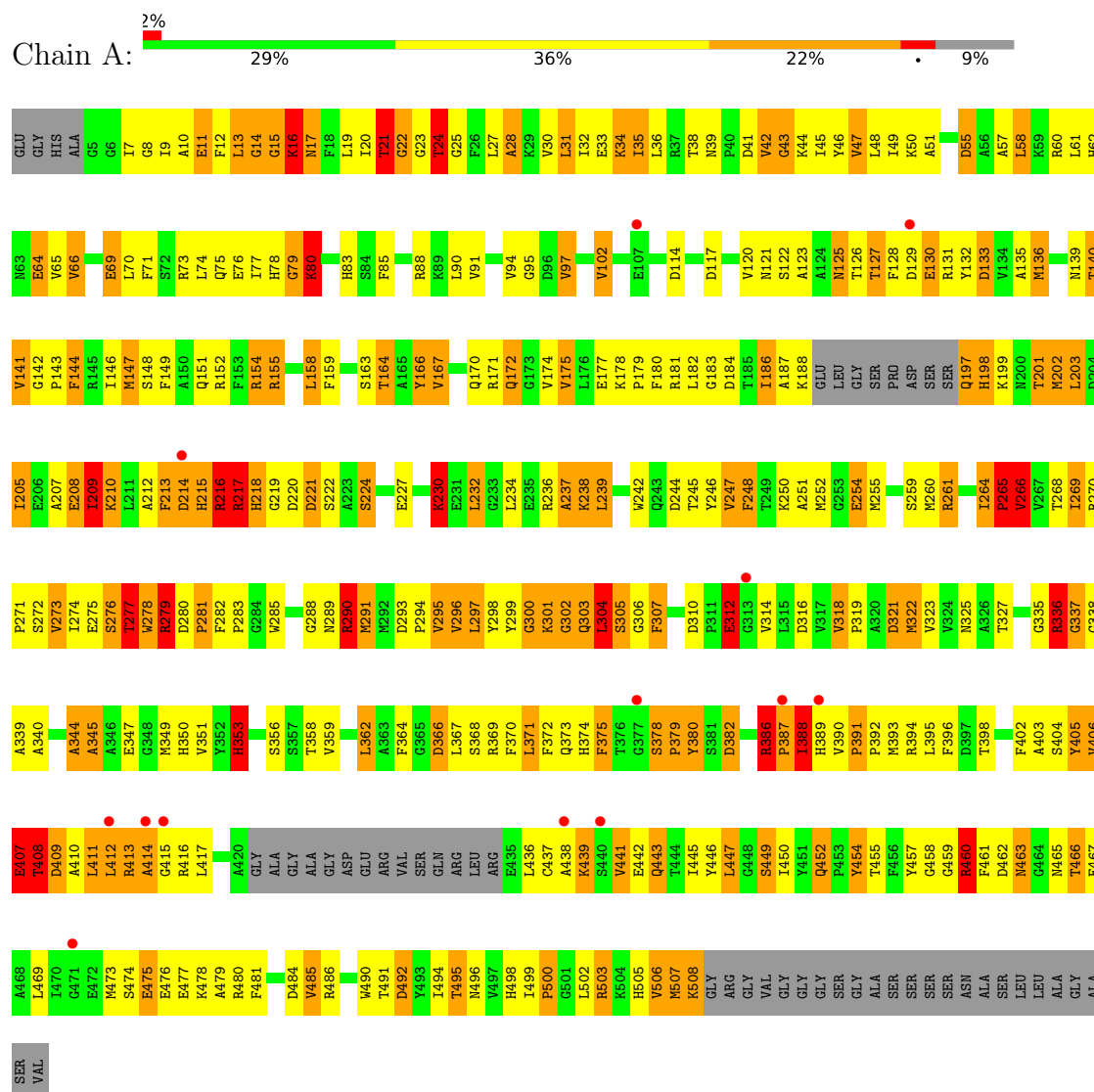
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	40	Total 40	O 40	0	0

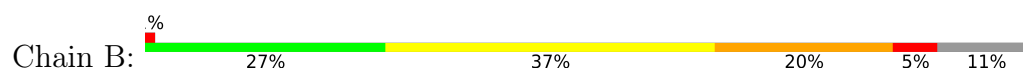
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fatty acyl-CoA reductase



• Molecule 1: Fatty acyl-CoA reductase



SER	G459	D397	A832	I269	L203	H136	V66	GLU
ASN	R460	T398	K333	R270	D204	M139	D67	GLY
ALA	N463	M399	E400	S271	I205	T140	T68	HIS
SER	N464	E401	R336	S272	E208	V141	B69	ALA
LEU	N465	F402	G337	V273	L209	G142	L70	G5
ALA	N466	A403	G338	L274	K210	P143	R73	G6
GLY	E467	S404	A839	E275	L211	F144	L74	I7
ALA	A468	Y405	A340	S276	A212	R145	Q75	G8
SER	L469	V406	A341	T277	F213	I146	L75	I9
VAL	I470	E407	A342	W278	D214	R147	E76	
	G471	I468	A343	W279	H215	S148	I77	L13
	E472	D409	A344	D280	H216		H78	G14
	M473	A410	A345	F281	R217	A152	G79	G15
	S474	L411	A346	F282	R218	F153	K80	K16
	E475	L412	E347	P283	H218	R154	D81	N17
	E476	G348	G348	G284	G219	R154	Y82	F18
	E477	R413	M349	W285	D220	R155	H83	L19
	E478	A414	H350	M286	D221	L156	I20	I20
	K478	G415	V851	E287	S222	K157	S84	T21
	A479	R416	Y352		A223	L158	R88	G22
	R480	L417	H353	R290	S224	F159	R89	G23
	F481	A418	V354	M291	F225	L160	L90	T24
	H482	GLY		M292	S226		G95	G25
	F483	ALA	V359	D293	E227	S163	D96	F26
	D484	GLY	N360	P294	E228	T164	L27	L27
	V485	ALA	P361	V295	M229	A165	A28	A28
	R486	GLY	A363	V296	K230	V167	R29	R29
		ALA	L362	L297	E231		V30	V30
		GLY	F364	Y298	L232		M101	L31
		ASP	G365	Y299		R171	V102	L32
	T491	GLU	D366	G300	E235		A105	E33
	D492	ARG	L367	K301	R236		P106	K34
	Y493	VAL	S368	G302	A237		E107	L35
	I494	SER	R369	Q303	K238		L108	L36
	T495	GLN	F370	L304	L239		A109	R37
	N496	ARG	L371	S305	E177		G110	T38
	V497	LEU	F372	F307	Q242		V111	N39
	H498	GLU	Q373	L308	D244		I112	P40
	I499	LEU		A309	T245		A113	D41
	P500	GLU	T376	D310	Y246		D114	V42
	G501	LEU	G377	P311	V247		E115	G43
	L502	C437	S378	E312	F248		V116	K44
	R503	A438	P379		T249		D117	I45
	K504	K439	Y380		K250		I118	Y46
	H505	S440	S381	L315	A251		I119	V47
	V506	V441	D382		M252		N120	L48
	M507		A383	V318	G253		N121	I49
	GLY	I445	A384	P319	E254		S122	K50
	ARG	Y446	G385	A320	M255		A123	A51
	GLY	L447	R386	D321	N258		R125	
	VAL	G448	P387	M322	M260		T126	D85
	GLY	S449	I388	V323	R261		E130	L58
	GLY	I450	H389	V324	G262		R131	L61
	GLY	Y451	V390	N325	C263		Y132	H62
	GLY	Q452	P391	A326	D264		D133	N63
	SER	P453	P392	G326	I264		T134	E64
	GLY	Y454	R392	L328	P265		A135	V65
	ALA	T455	M393	S329				
	SER	F456	R394	S330				
	SER	Y457	L395	M331				
	SER	G458	F396					

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	222.81Å 222.81Å 114.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.40 48.45 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.45-3.40) 97.7 (48.45-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.21 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.240 0.216 , 0.227	Depositor DCC
R_{free} test set	2223 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 174.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: NAP

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	1.15	7/3833 (0.2%)	2.19	116/5180 (2.2%)
1	B	1.21	13/3761 (0.3%)	2.26	140/5085 (2.8%)
All	All	1.18	20/7594 (0.3%)	2.22	256/10265 (2.5%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	PRO	N-CD	15.57	1.69	1.47
1	B	392	PRO	N-CD	10.07	1.61	1.47
1	A	339	ALA	CA-C	-9.81	1.40	1.52
1	B	22	GLY	C-O	8.73	1.35	1.23
1	B	483	PHE	CA-C	8.62	1.64	1.53

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	PHE	N-CA-C	32.90	153.26	112.47
1	B	66	VAL	N-CA-C	-25.29	74.56	109.46
1	B	382	ASP	N-CA-C	-24.88	73.56	110.14
1	B	392	PRO	N-CA-C	-24.38	74.80	111.13
1	B	391	PRO	N-CA-C	-24.33	81.02	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3753	0	3712	509	2
1	B	3682	0	3639	465	2
2	A	48	0	25	10	0
2	B	48	0	25	3	0
3	A	45	0	0	38	0
3	B	40	0	0	30	0
All	All	7616	0	7401	948	2

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 63.

The worst 5 of 948 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:A:215:HIS:CD2	1:B:216:ARG:HG2	1.26	1.69
1:B:306:GLY:HA2	1:B:393:MET:CE	1.26	1.59
1:B:446:TYR:CE1	1:B:450:ILE:HD11	1.43	1.51
1:B:446:TYR:HE1	1:B:450:ILE:CD1	1.25	1.50
1:A:215:HIS:CD2	1:B:216:ARG:CG	1.94	1.47

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:CB	1:B:303:GLN:OE1[5_554]	1.82	0.38
1:A:416:ARG:NH2	1:B:437:CYS:O[5_554]	2.15	0.05

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	476/532 (90%)	375 (79%)	91 (19%)	10 (2%)	5	24
1	B	467/532 (88%)	391 (84%)	68 (15%)	8 (2%)	7	28
All	All	943/1064 (89%)	766 (81%)	159 (17%)	18 (2%)	6	26

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	ASP
1	B	296	VAL
1	A	442	GLU
1	A	75	GLN
1	A	144	PHE

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	391/422 (93%)	277 (71%)	114 (29%)	0	1
1	B	384/422 (91%)	276 (72%)	108 (28%)	0	1
All	All	775/844 (92%)	553 (71%)	222 (29%)	0	1

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	THR
1	B	508	LYS
1	B	152	ARG
1	B	502	LEU
1	B	409	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	401	GLN
1	B	465	ASN
1	B	463	ASN
1	A	350	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	NAP	B	601	-	50,52,52	1.06	2 (4%)	71,80,80	1.78	15 (21%)
2	NAP	A	601	-	50,52,52	0.94	2 (4%)	71,80,80	1.65	11 (15%)

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	NAP	B	601	-	-	21/35/67/67	0/5/5/5
2	NAP	A	601	-	-	15/35/67/67	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	NAP	C2N-N1N	5.91	1.41	1.35
2	A	601	NAP	C2N-N1N	4.51	1.39	1.35
2	A	601	NAP	O4D-C1D	3.17	1.45	1.40
2	B	601	NAP	P2B-O2B	2.33	1.63	1.59

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAP	C6N-N1N-C2N	-6.51	116.34	121.88
2	B	601	NAP	P2B-O2B-C2B	-6.08	107.20	123.43
2	B	601	NAP	O2X-P2B-O2B	5.25	126.30	105.85
2	B	601	NAP	O2B-P2B-O1X	-4.51	93.25	109.33
2	A	601	NAP	C5N-C4N-C3N	-4.36	116.08	120.36

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAP	C5B-O5B-PA-O3
2	A	601	NAP	O4B-C4B-C5B-O5B
2	A	601	NAP	C3B-C4B-C5B-O5B
2	A	601	NAP	C5D-O5D-PN-O3
2	A	601	NAP	C5D-O5D-PN-O2N

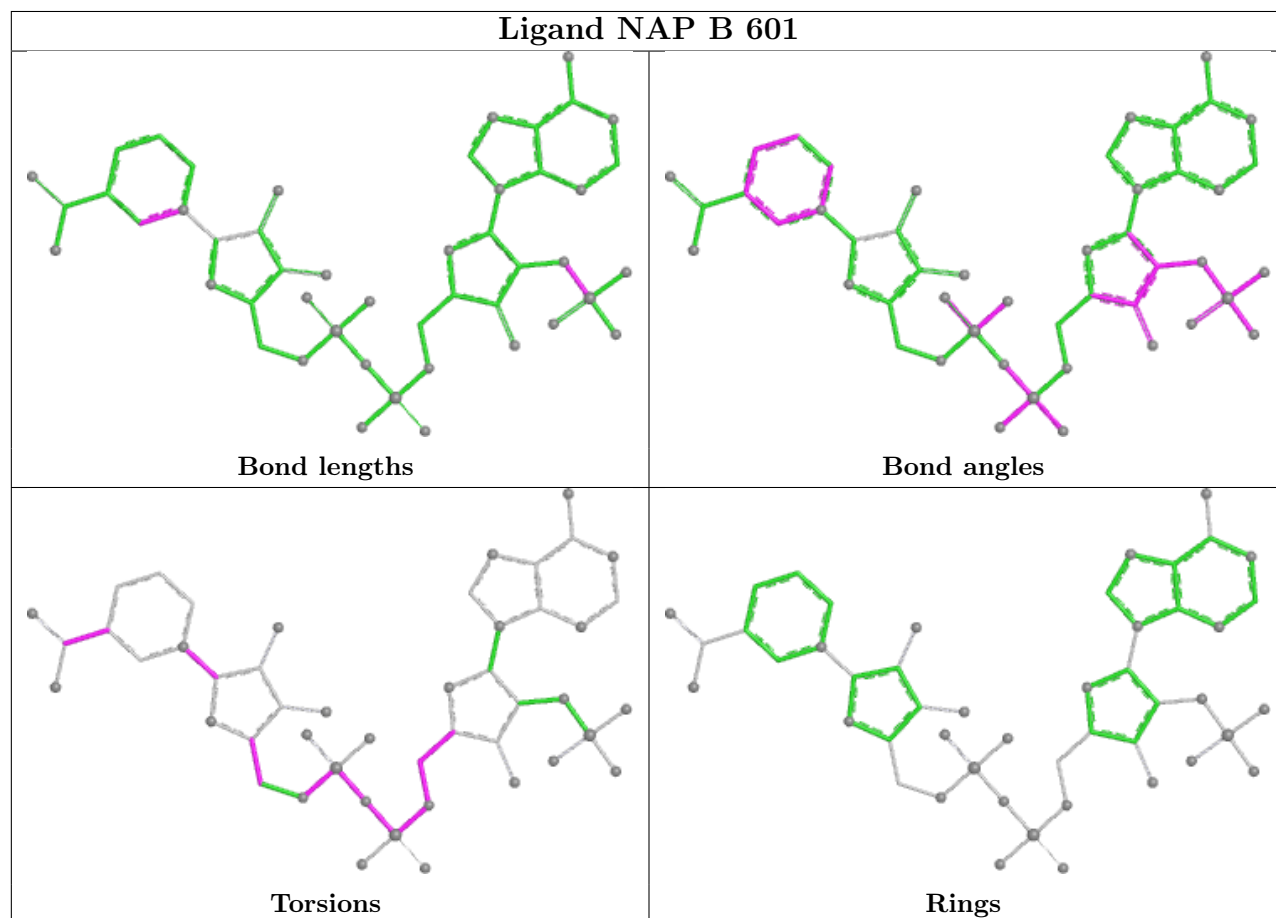
There are no ring outliers.

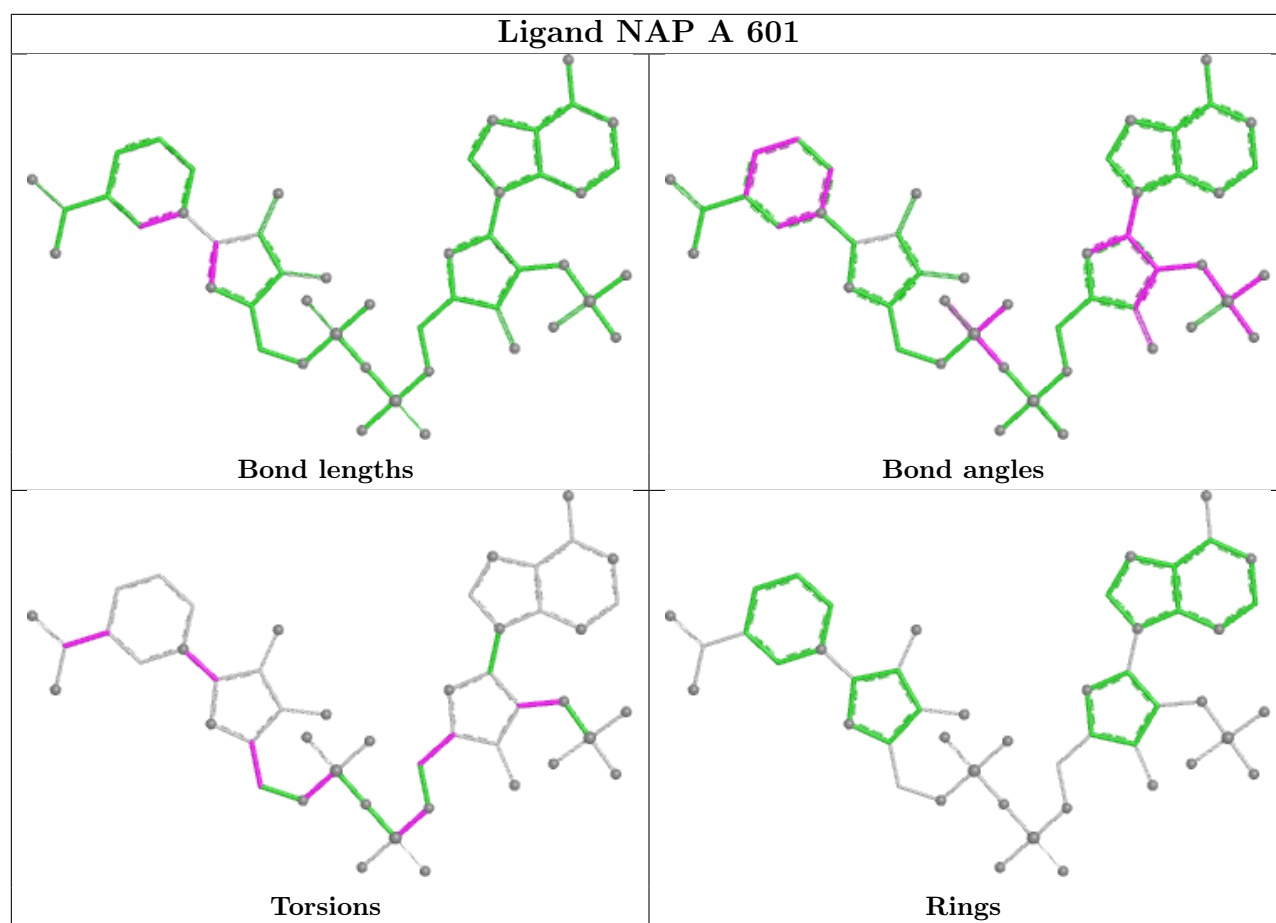
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAP	3	0
2	A	601	NAP	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	482/532 (90%)	0.08	13 (2%) 56 42	30, 97, 152, 190	0
1	B	473/532 (88%)	0.05	7 (1%) 72 57	60, 95, 144, 195	0
All	All	955/1064 (89%)	0.07	20 (2%) 63 48	30, 96, 149, 195	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	GLY	3.8
1	B	216	ARG	3.8
1	A	387	PRO	3.4
1	A	414	ALA	3.2
1	A	415	GLY	3.0

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

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

6.3 Carbohydrates [i](#)

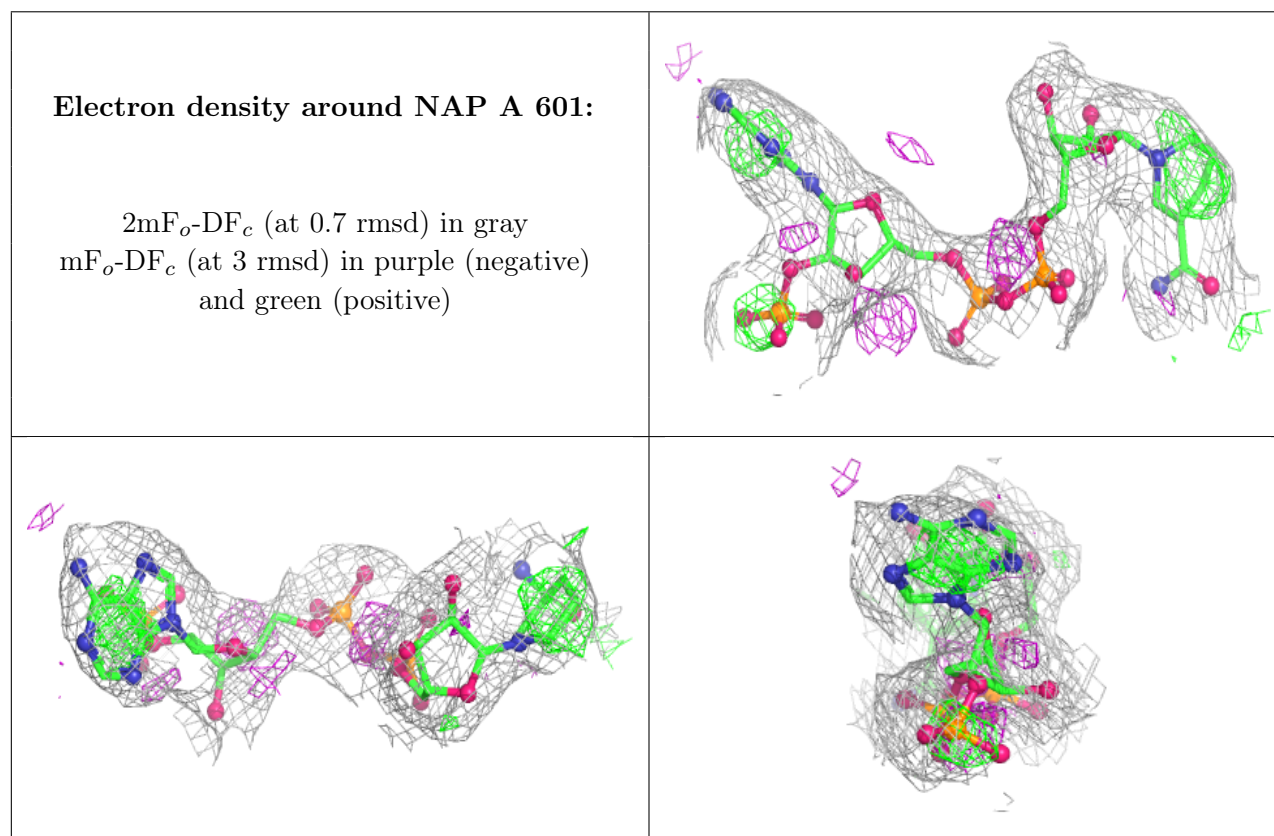
There are no oligosaccharides in this entry.

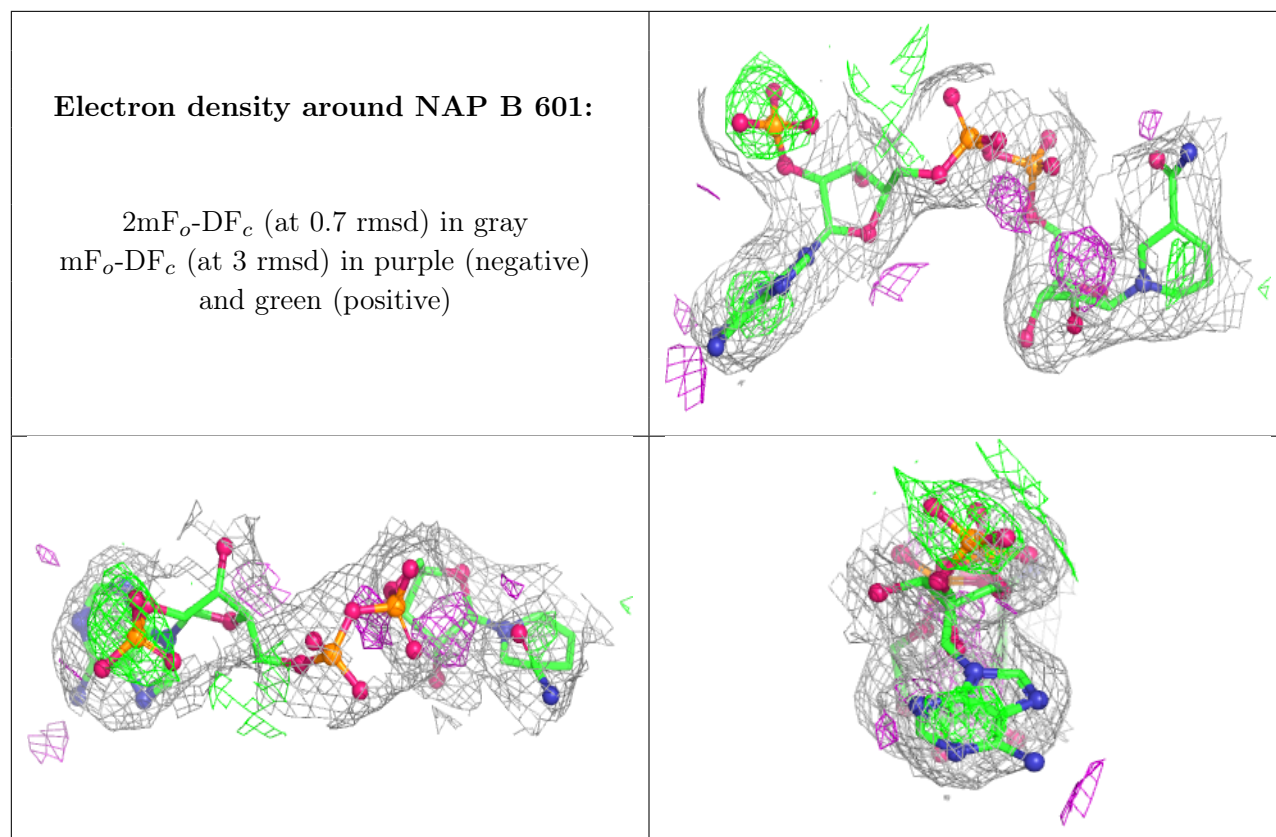
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	NAP	A	601	48/48	0.98	0.09	65,80,113,136	0
2	NAP	B	601	48/48	0.98	0.09	55,81,112,122	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.