



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:22 PM UTC

PDB ID : 4WDT / pdb_00004wdt
Title : 17beta-HSD5 in complex with 2-nitro-5-(phenylsulfonyl)phenol
Authors : Amano, Y.; Yamaguchi, T.
Deposited on : 2014-09-09
Resolution : 1.50 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

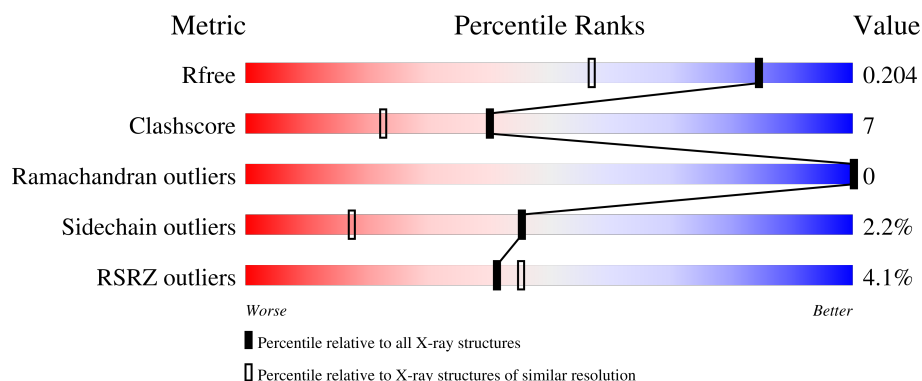
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	331	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2798 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 Aldo-keto reductase family 1 member C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2524	1609	440	463	12			

There are 9 discrepancies between the modelled and reference sequences:

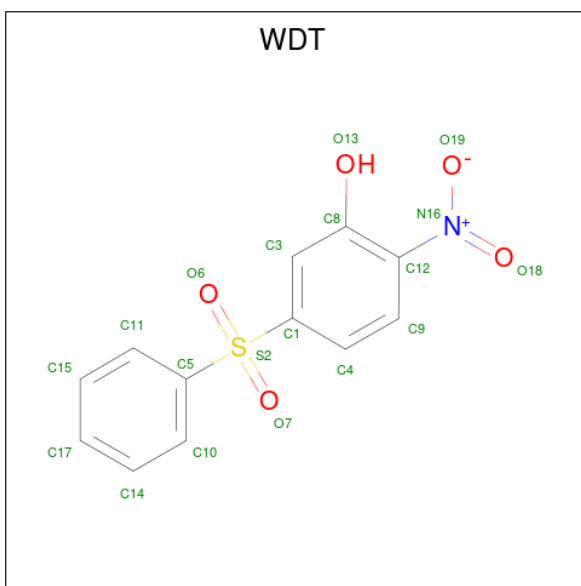
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLN	HIS	variant	UNP P42330
A	324	LEU	-	expression tag	UNP P42330
A	325	GLU	-	expression tag	UNP P42330
A	326	HIS	-	expression tag	UNP P42330
A	327	HIS	-	expression tag	UNP P42330
A	328	HIS	-	expression tag	UNP P42330
A	329	HIS	-	expression tag	UNP P42330
A	330	HIS	-	expression tag	UNP P42330
A	331	HIS	-	expression tag	UNP P42330

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is 2-nitro-5-(phenylsulfonyl)phenol (CCD ID: WDT) (formula: $C_{12}H_9NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	12	1	5	1		

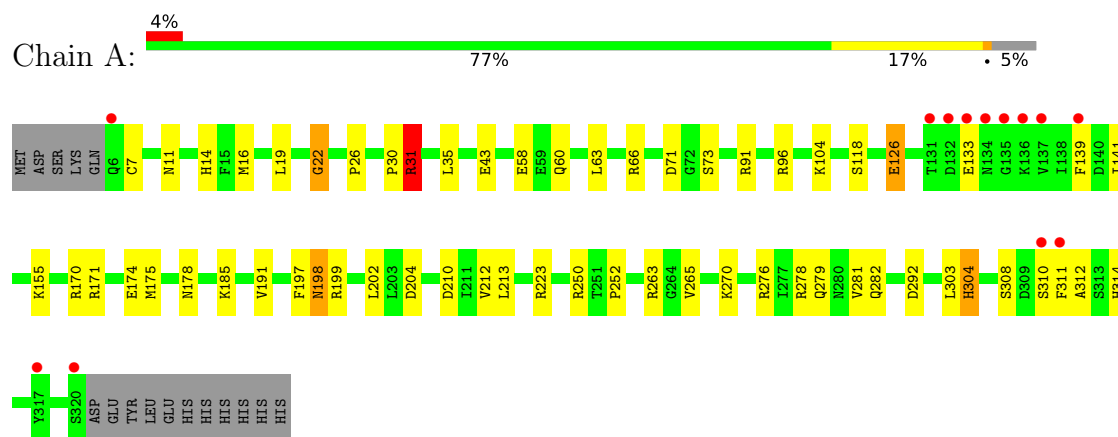
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	207	Total 207	O 207	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: Aldo-keto reductase family 1 member C3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.51Å 62.56Å 96.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.13 – 1.50 38.13 – 1.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (38.13-1.50) 91.5 (38.13-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.176 , 0.204 0.175 , 0.204	Depositor DCC
R_{free} test set	2540 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	10.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2798	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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: WDT, 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	1.59	17/2582 (0.7%)	1.49	28/3494 (0.8%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CD-OE1	14.49	1.52	1.25
1	A	22	GLY	C-O	6.05	1.30	1.24
1	A	265	VAL	N-CA	5.95	1.53	1.46
1	A	191	VAL	N-CA	5.88	1.52	1.46
1	A	310	SER	CA-C	-5.84	1.45	1.52
1	A	155	LYS	C-O	-5.50	1.17	1.24
1	A	212	VAL	C-O	-5.45	1.17	1.24
1	A	63	LEU	N-CA	5.40	1.52	1.46
1	A	276	ARG	CD-NE	-5.34	1.38	1.46
1	A	26	PRO	CA-C	5.30	1.57	1.52
1	A	58	GLU	CG-CD	5.30	1.65	1.52
1	A	304	HIS	C-O	5.28	1.30	1.24
1	A	252	PRO	N-CA	-5.25	1.40	1.47
1	A	11	ASN	N-CA	5.20	1.53	1.46
1	A	175	MET	N-CA	-5.11	1.40	1.46
1	A	16	MET	CA-C	5.03	1.58	1.52
1	A	7	CYS	N-CA	5.01	1.52	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ARG	NE-CZ-NH1	-16.05	105.45	121.50
1	A	276	ARG	NE-CZ-NH2	15.67	133.30	119.20
1	A	31	ARG	NE-CZ-NH2	11.55	129.59	119.20
1	A	31	ARG	NE-CZ-NH1	-10.87	110.63	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	GLU	CG-CD-OE2	-9.10	97.46	118.40
1	A	31	ARG	CD-NE-CZ	8.69	136.56	124.40
1	A	185	LYS	CA-C-N	-7.41	112.13	119.76
1	A	185	LYS	C-N-CA	-7.41	112.13	119.76
1	A	58	GLU	CG-CD-OE1	6.65	133.69	118.40
1	A	96	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	A	19	LEU	CA-C-N	-6.34	117.81	122.18
1	A	19	LEU	C-N-CA	-6.34	117.81	122.18
1	A	263	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	A	263	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	31	ARG	CG-CD-NE	-5.87	99.08	112.00
1	A	118	SER	N-CA-CB	-5.86	104.95	111.10
1	A	66	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	A	292	ASP	N-CA-C	-5.75	104.92	111.07
1	A	276	ARG	CD-NE-CZ	5.53	132.15	124.40
1	A	213	LEU	CD1-CG-CD2	-5.43	98.86	110.80
1	A	312	ALA	N-CA-C	-5.40	105.95	112.54
1	A	223	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	263	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	A	314	HIS	CA-C-N	-5.23	114.22	119.56
1	A	314	HIS	C-N-CA	-5.23	114.22	119.56
1	A	14	HIS	CA-C-O	-5.17	116.00	121.94
1	A	91	ARG	CG-CD-NE	-5.06	100.86	112.00
1	A	199	ARG	NE-CZ-NH2	5.05	123.75	119.20

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	2524	0	2531	34	0
2	A	48	0	25	3	0
3	A	19	0	8	2	0
4	A	207	0	0	8	0
All	All	2798	0	2564	34	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (34) 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:139:PHE:CE1	1:A:141:ILE:HD11	1.68	1.27
1:A:210:ASP:HB3	4:A:561:HOH:O	1.40	1.22
1:A:60:GLN:HG2	4:A:654:HOH:O	1.41	1.20
1:A:31:ARG:HD2	1:A:31:ARG:N	1.66	1.03
1:A:60:GLN:CG	4:A:654:HOH:O	2.01	1.02
1:A:139:PHE:HE1	1:A:141:ILE:HD11	1.07	0.99
1:A:139:PHE:CE1	1:A:141:ILE:CD1	2.51	0.92
1:A:139:PHE:HE1	1:A:141:ILE:CD1	1.85	0.89
1:A:204:ASP:CG	4:A:696:HOH:O	2.25	0.79
1:A:204:ASP:CB	4:A:696:HOH:O	2.31	0.79
1:A:31:ARG:N	1:A:31:ARG:CD	2.47	0.77
1:A:204:ASP:HB3	4:A:696:HOH:O	1.86	0.74
1:A:198:ASN:C	1:A:198:ASN:HD22	2.02	0.67
1:A:43:GLU:HG2	4:A:703:HOH:O	1.95	0.66
1:A:126:GLU:H	1:A:126:GLU:CD	2.04	0.65
1:A:174:GLU:OE1	1:A:178:ASN:ND2	2.29	0.64
1:A:71:ASP:OD1	1:A:73:SER:OG	2.22	0.56
1:A:311:PHE:CZ	3:A:402:WDT:H2	2.41	0.55
1:A:250:ARG:HH21	1:A:282:GLN:HE21	1.56	0.53
1:A:30:PRO:C	1:A:31:ARG:HD2	2.32	0.52
1:A:35:LEU:HB2	1:A:60:GLN:HE21	1.75	0.52
1:A:279:GLN:NE2	2:A:401:NAP:H62A	2.07	0.51
1:A:133:GLU:HA	1:A:133:GLU:OE1	2.12	0.50
1:A:270:LYS:O	2:A:401:NAP:H8A	2.13	0.48
1:A:278:ARG:O	1:A:281:VAL:HG22	2.14	0.47
1:A:197:PHE:CE2	1:A:304:HIS:HB3	2.52	0.45
1:A:22:GLY:HA3	2:A:401:NAP:H4D	1.99	0.44
1:A:170:ARG:HG3	1:A:202:LEU:HD13	2.01	0.43
1:A:250:ARG:NH2	1:A:282:GLN:HE21	2.16	0.43
1:A:139:PHE:CD1	1:A:141:ILE:CD1	3.01	0.42
1:A:308:SER:HB3	1:A:311:PHE:CE2	2.55	0.42
1:A:60:GLN:HG3	4:A:654:HOH:O	1.93	0.41
1:A:250:ARG:HH21	1:A:282:GLN:NE2	2.17	0.41
1:A:311:PHE:CE1	3:A:402:WDT:H2	2.55	0.41

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	313/331 (95%)	304 (97%)	9 (3%)	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	279/295 (95%)	273 (98%)	6 (2%)	45	17

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	104	LYS
1	A	126	GLU
1	A	171	ARG
1	A	198	ASN
1	A	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	60	GLN

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Mol	Chain	Res	Type
1	A	198	ASN
1	A	222	GLN
1	A	279	GLN
1	A	282	GLN

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	A	401	-	50,52,52	1.06	2 (4%)	71,80,80	1.06	4 (5%)
3	WDT	A	402	-	20,20,20	1.03	0	25,29,29	3.51	13 (52%)

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	A	401	-	-	3/35/67/67	0/5/5/5
3	WDT	A	402	-	-	4/14/16/16	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	PA-O3	3.22	1.63	1.59
2	A	401	NAP	C8A-N9A	2.90	1.42	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	WDT	C3-C8-C12	7.02	123.02	118.04
3	A	402	WDT	O7-S2-C1	-6.64	99.79	107.96
3	A	402	WDT	O6-S2-C5	-5.77	100.85	107.96
3	A	402	WDT	C3-C1-S2	-5.41	111.95	119.15
3	A	402	WDT	O6-S2-C1	5.30	114.47	107.96
3	A	402	WDT	C11-C5-S2	4.93	125.92	119.49
3	A	402	WDT	O7-S2-O6	4.66	128.67	119.25
3	A	402	WDT	C15-C17-C14	-3.88	114.55	119.87
3	A	402	WDT	C10-C5-S2	-3.66	114.73	119.49
3	A	402	WDT	C4-C1-C3	3.65	125.19	120.68
3	A	402	WDT	C17-C15-C11	3.16	124.13	120.24
3	A	402	WDT	C17-C14-C10	2.79	123.67	120.24
3	A	402	WDT	C4-C1-S2	2.59	122.86	119.49
2	A	401	NAP	C2B-C3B-C4B	2.32	106.97	101.99
2	A	401	NAP	C2A-N1A-C6A	2.29	122.50	118.73
2	A	401	NAP	C2B-C1B-N9A	-2.12	110.27	113.75
2	A	401	NAP	O7N-C7N-C3N	2.09	122.16	119.60

There are no chirality outliers.

All (7) torsion outliers are listed below:

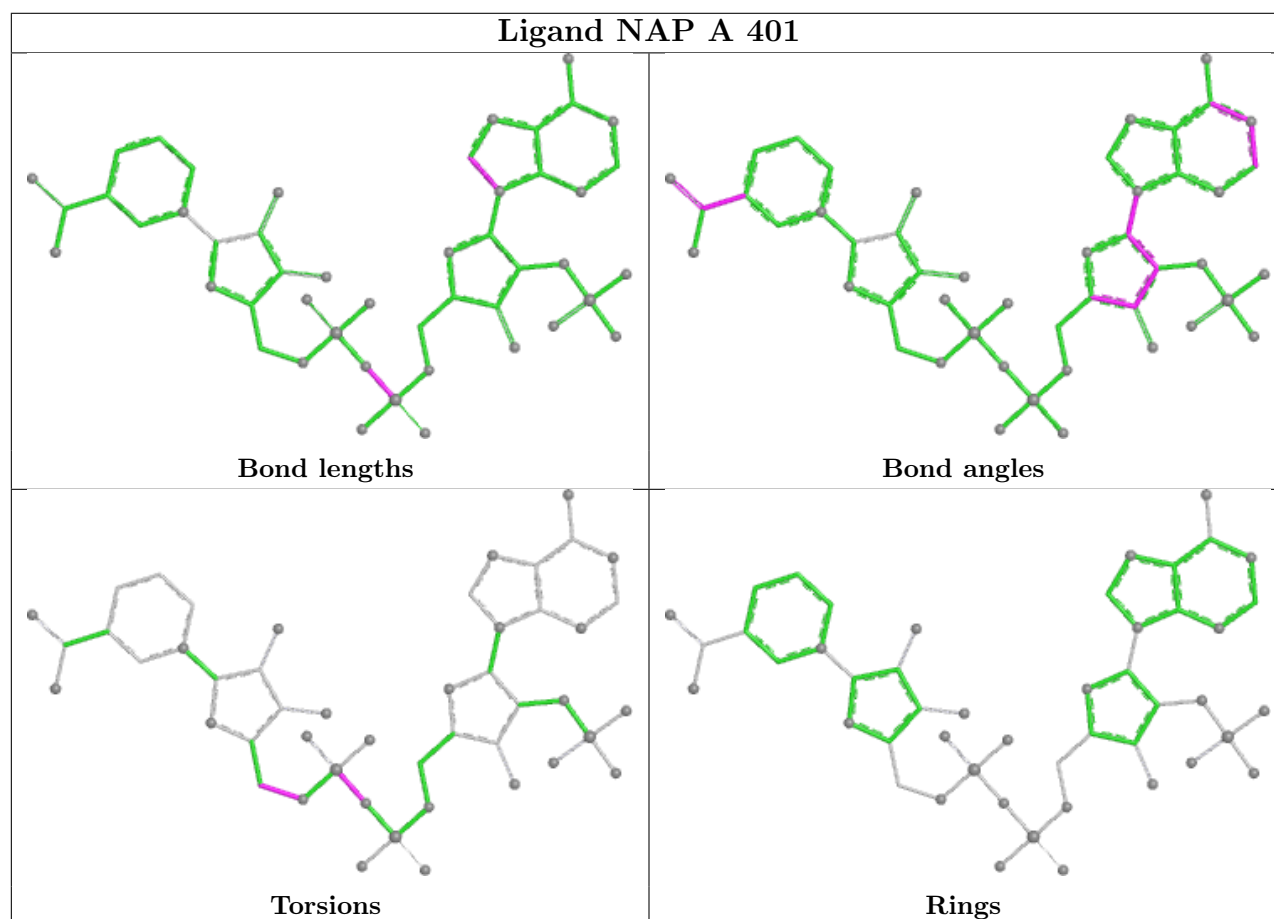
Mol	Chain	Res	Type	Atoms
3	A	402	WDT	C11-C5-S2-O6
2	A	401	NAP	PA-O3-PN-O5D
3	A	402	WDT	C10-C5-S2-O6
2	A	401	NAP	C4D-C5D-O5D-PN
3	A	402	WDT	C11-C5-S2-C1
3	A	402	WDT	C10-C5-S2-C1
2	A	401	NAP	PA-O3-PN-O2N

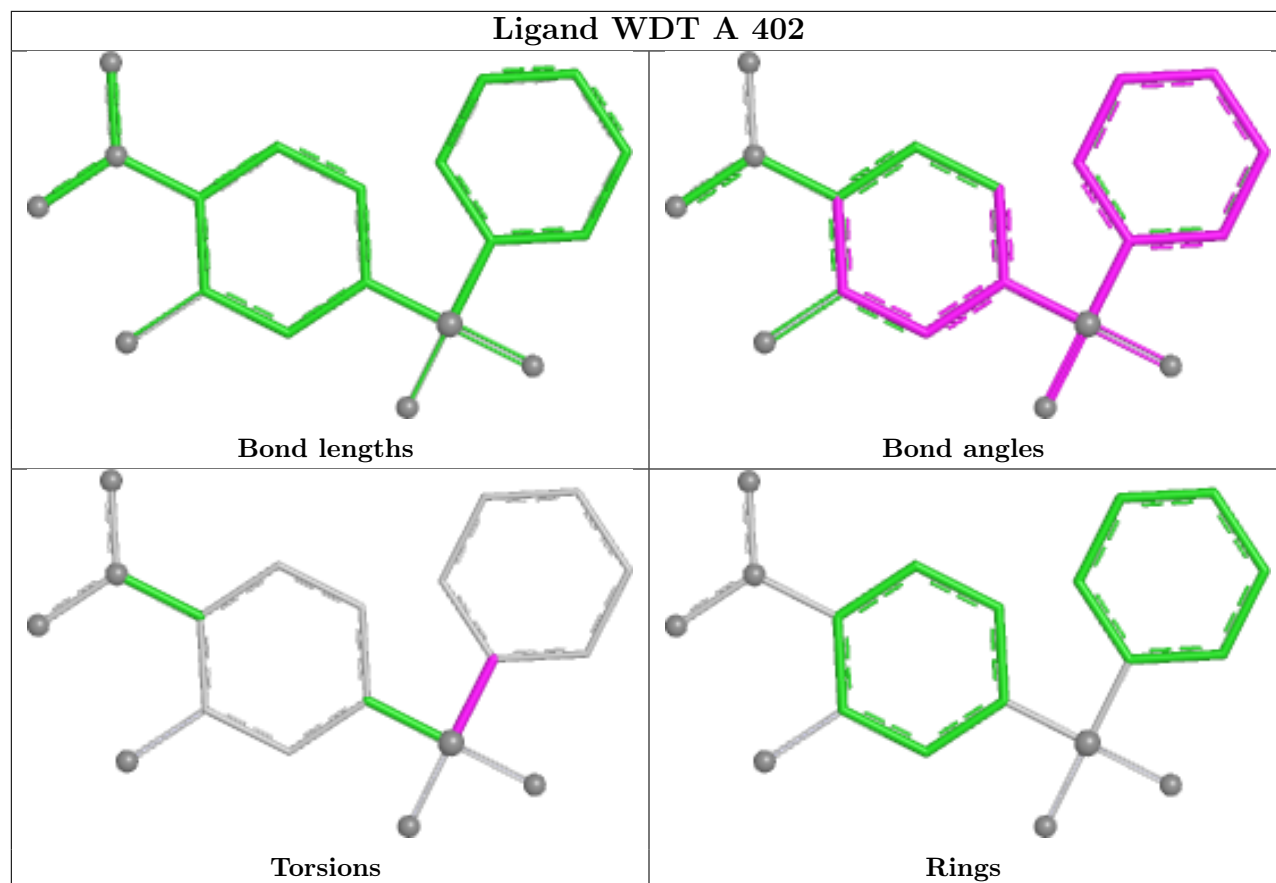
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	3	0
3	A	402	WDT	2	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	315/331 (95%)	-0.15	13 (4%) 41 45	5, 10, 26, 58	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	5.3
1	A	135	GLY	4.2
1	A	134	ASN	3.3
1	A	131	THR	3.1
1	A	133	GLU	3.0
1	A	311	PHE	2.8
1	A	132	ASP	2.5
1	A	139	PHE	2.5
1	A	310	SER	2.4
1	A	6	GLN	2.2
1	A	136	LYS	2.0
1	A	317	TYR	2.0
1	A	320	SER	2.0

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](#)

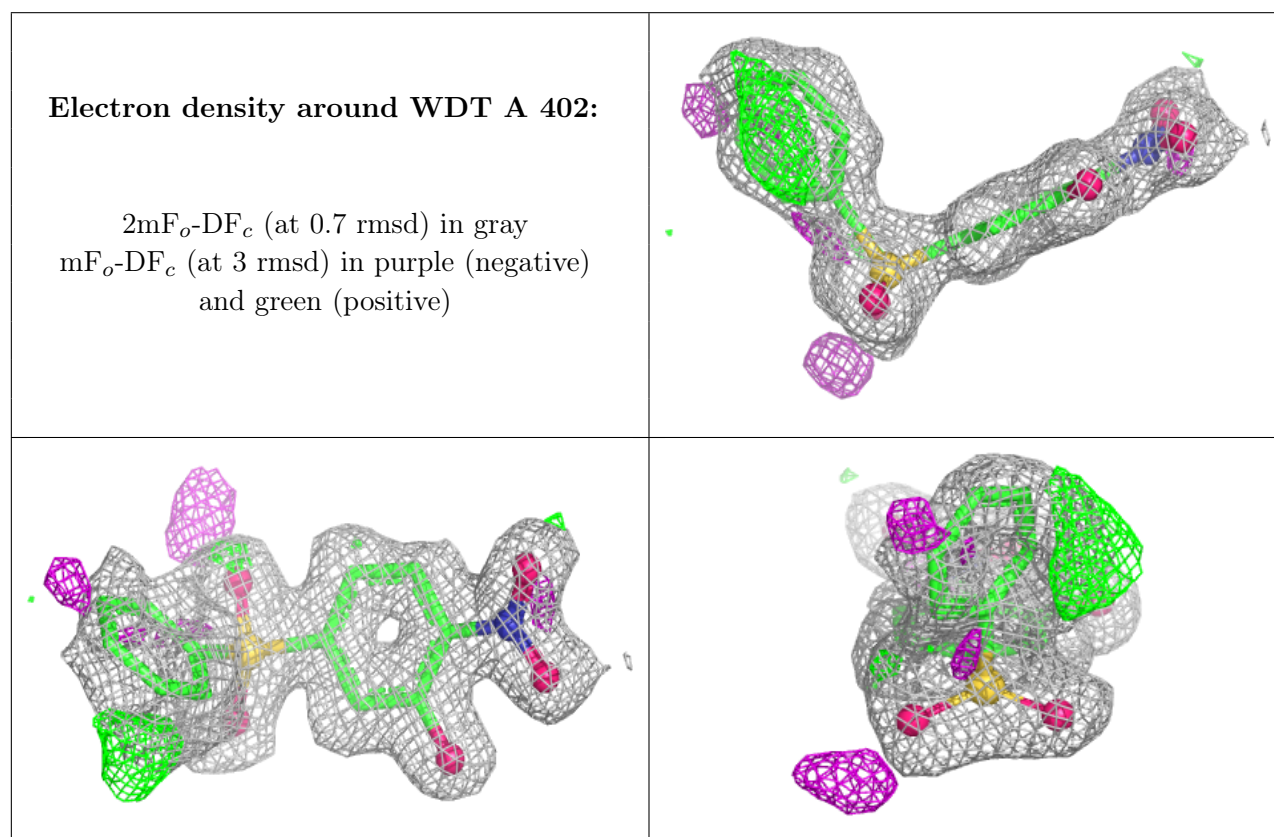
There are no oligosaccharides in this entry.

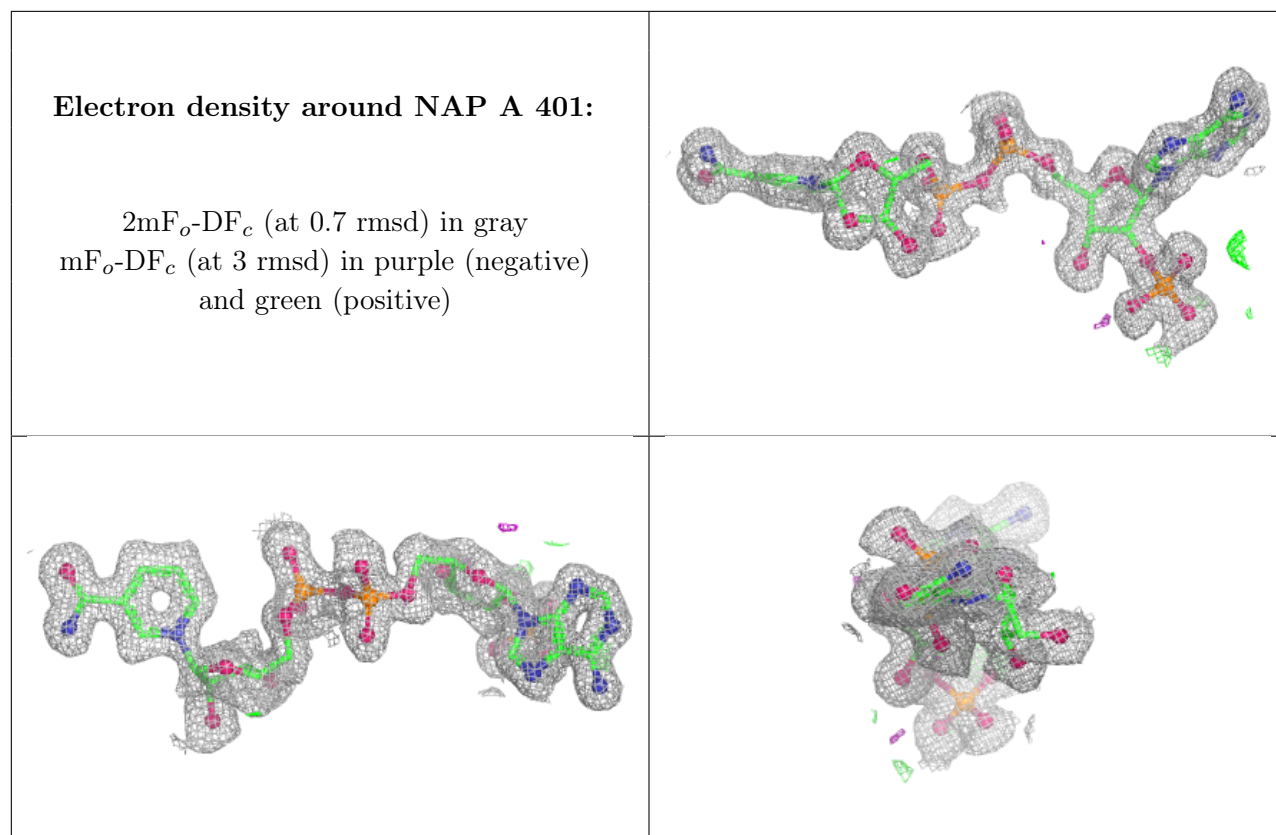
6.4 Ligands ⓘ

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	WDT	A	402	19/19	0.94	0.10	10,15,25,27	0
2	NAP	A	401	48/48	0.99	0.04	5,6,9,10	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.