



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:20 PM UTC

PDB ID : 4PVD / pdb_00004pvd
Title : Crystal structure of yeast methylglyoxal/isovaleraldehyde reductase Gre2 complexed with NADPH
Authors : Guo, P.C.; Bao, Z.Z.; Li, W.F.; Zhou, C.Z.
Deposited on : 2014-03-17
Resolution : 2.40 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

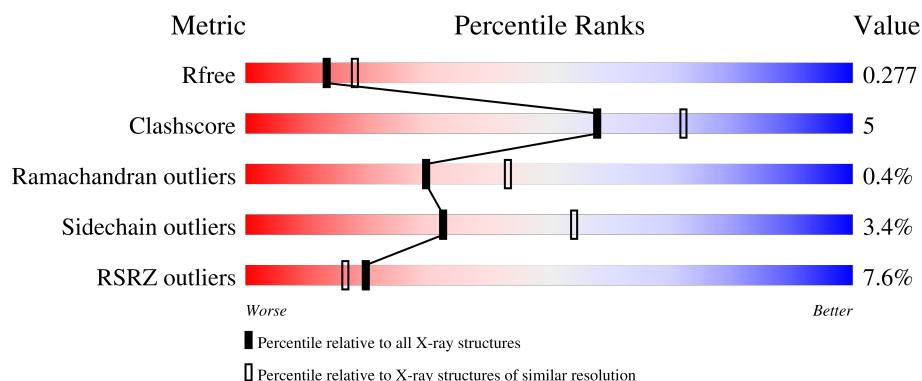
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

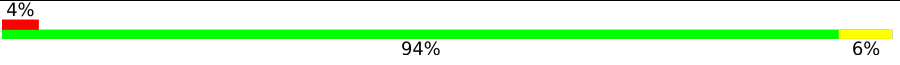
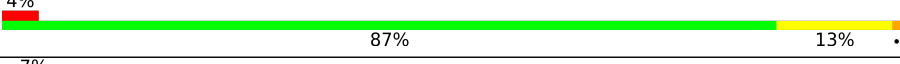
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

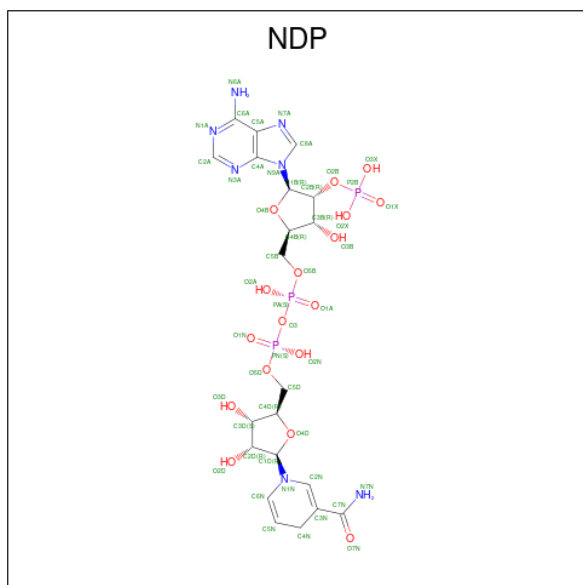
Mol	Chain	Length	Quality of chain
1	A	342	
1	B	342	
1	C	342	
1	D	342	

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 NADPH-dependent methylglyoxal reductase GRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total 2690	C 1714	N 452	O 514	S 10	0	0	0
1	B	342	Total 2690	C 1714	N 452	O 514	S 10	0	0	0
1	C	308	Total 2422	C 1551	N 409	O 456	S 6	0	0	0
1	D	305	Total 2391	C 1531	N 405	O 449	S 6	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

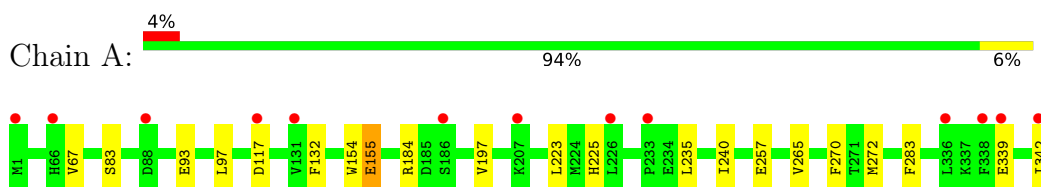
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total 40	O 40	0	0
3	B	39	Total 39	O 39	0	0
3	C	28	Total 28	O 28	0	0
3	D	20	Total 20	O 20	0	0

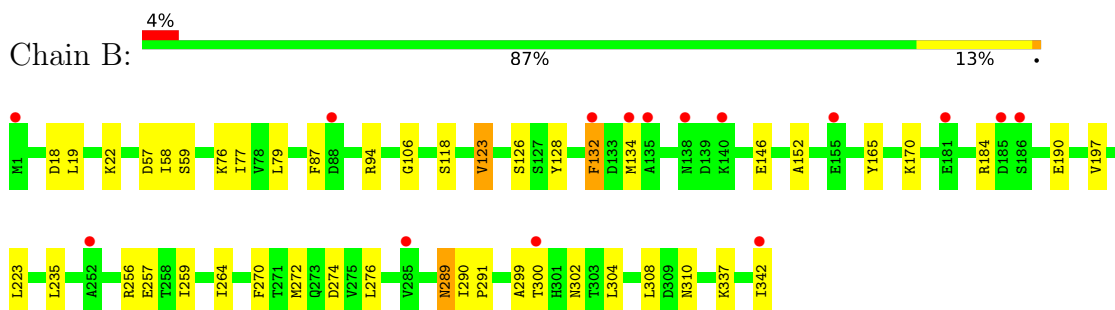
3 Residue-property plots [i](#)

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

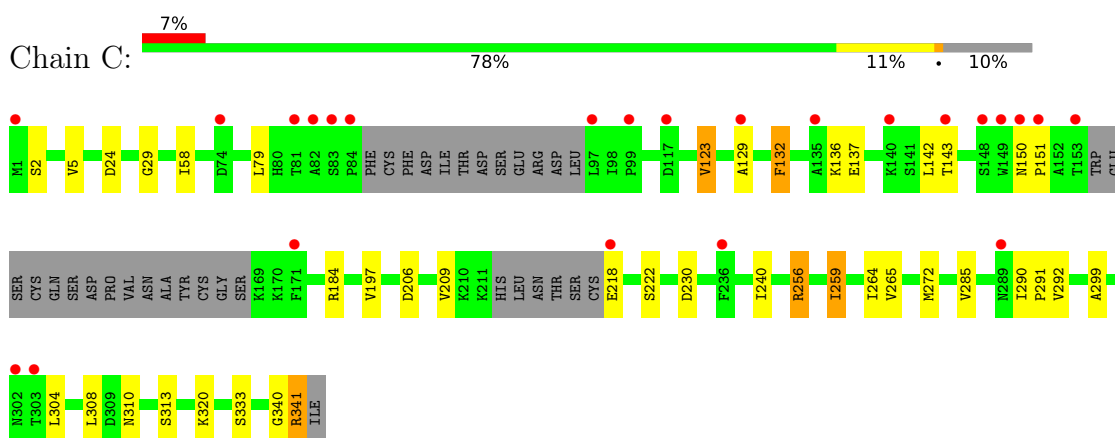
- Molecule 1: NADPH-dependent methylglyoxal reductase GRE2



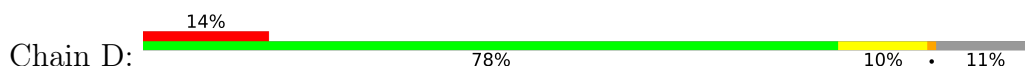
- Molecule 1: NADPH-dependent methylglyoxal reductase GRE2

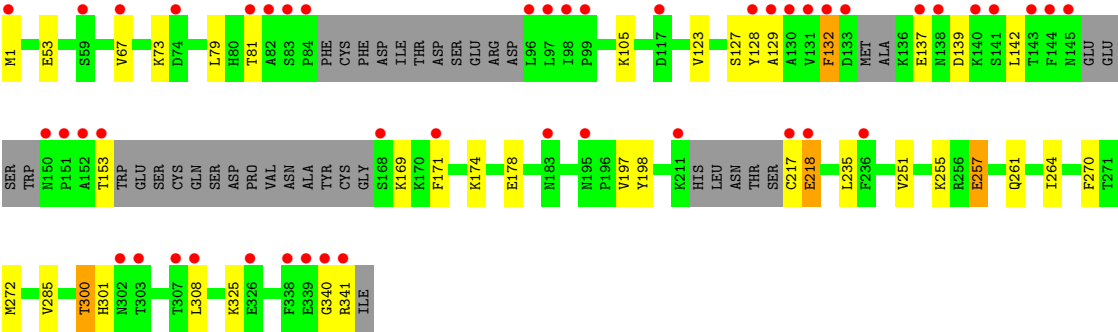


- Molecule 1: NADPH-dependent methylglyoxal reductase GRE2



- Molecule 1: NADPH-dependent methylglyoxal reductase GRE2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.31Å 92.89Å 201.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 99.3 (50.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.242 , 0.288 0.237 , 0.277	Depositor DCC
R_{free} test set	3358 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10416	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6663e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NDP

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	0.47	0/2745	0.81	2/3705 (0.1%)
1	B	0.46	0/2745	0.82	0/3705
1	C	0.46	0/2467	0.79	0/3322
1	D	0.47	0/2432	0.80	0/3271
All	All	0.47	0/10389	0.81	2/14003 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	PHE	CA-C-N	5.25	125.05	119.28
1	A	283	PHE	C-N-CA	5.25	125.05	119.28

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	2690	0	2679	11	0
1	B	2690	0	2679	34	0
1	C	2422	0	2444	24	0
1	D	2391	0	2422	24	0
2	A	48	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	26	3	0
3	A	40	0	0	0	0
3	B	39	0	0	2	0
3	C	28	0	0	0	0
3	D	20	0	0	0	0
All	All	10416	0	10276	93	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 5.

All (93) 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:C:136:LYS:HB3	1:C:142:LEU:HD22	1.19	1.16
1:C:136:LYS:HB3	1:C:142:LEU:CD2	1.79	1.12
1:D:139:ASP:OD2	1:D:142:LEU:HD13	1.66	0.95
1:C:136:LYS:HD3	1:C:142:LEU:HD21	1.57	0.84
1:A:235:LEU:HD23	1:A:272:MET:HE3	1.61	0.81
1:B:256:ARG:O	1:B:259:ILE:HG12	1.85	0.76
1:B:289:ASN:N	1:B:289:ASN:HD22	1.84	0.76
1:B:270:PHE:HE1	1:B:272:MET:CE	1.97	0.76
1:C:340:GLY:O	1:C:341:ARG:HB2	1.84	0.75
1:D:139:ASP:OD2	1:D:142:LEU:CD1	2.39	0.71
1:D:217:CYS:O	1:D:218:GLU:HG3	1.92	0.70
1:B:235:LEU:HD23	1:B:272:MET:HE3	1.75	0.69
1:A:235:LEU:HD23	1:A:272:MET:CE	2.23	0.67
1:C:136:LYS:CB	1:C:142:LEU:CD2	2.67	0.67
1:C:218:GLU:HA	1:C:218:GLU:OE1	1.94	0.66
1:D:174:LYS:O	1:D:178:GLU:HG3	1.97	0.64
1:B:299:ALA:HA	1:B:304:LEU:HD13	1.79	0.64
1:A:154:TRP:O	1:A:155:GLU:HB2	1.98	0.63
1:B:79:LEU:CD2	1:B:123:VAL:HG13	2.29	0.62
1:B:87:PHE:HE1	1:B:165:TYR:HB2	1.63	0.62
1:D:127:SER:HB2	1:D:169:LYS:HD2	1.82	0.62
1:B:76:LYS:HG3	1:B:77:ILE:HG12	1.82	0.62
1:B:289:ASN:N	1:B:289:ASN:ND2	2.48	0.61
1:C:240:ILE:HG12	1:C:265:VAL:HG12	1.81	0.61
1:D:129:ALA:HA	1:D:132:PHE:CE1	2.37	0.60
1:B:79:LEU:HD23	1:B:123:VAL:HG13	1.83	0.59
1:B:184:ARG:NH2	1:B:190:GLU:OE1	2.36	0.59
1:B:337:LYS:HA	1:B:342:ILE:HD13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:GLU:HG3	1:D:67:VAL:HG23	1.85	0.58
1:B:132:PHE:CE2	1:B:134:MET:HB3	2.39	0.57
1:D:257:GLU:H	1:D:257:GLU:CD	2.12	0.57
1:C:136:LYS:HB3	1:C:142:LEU:HD21	1.78	0.56
1:B:270:PHE:HE1	1:B:272:MET:HE2	1.69	0.55
1:C:136:LYS:CD	1:C:142:LEU:HD21	2.32	0.54
1:A:270:PHE:HE1	1:A:272:MET:HE2	1.72	0.54
1:C:206:ASP:O	1:C:209:VAL:HG23	2.08	0.53
1:B:270:PHE:HE1	1:B:272:MET:HE1	1.70	0.53
1:B:94:ARG:NH1	1:D:325:LYS:HZ3	2.06	0.53
1:B:290:ILE:HB	1:B:291:PRO:HD2	1.90	0.52
1:D:340:GLY:O	1:D:341:ARG:HB2	2.09	0.52
1:D:79:LEU:HD23	1:D:123:VAL:HB	1.92	0.52
1:C:340:GLY:O	1:C:341:ARG:CB	2.58	0.52
1:C:299:ALA:HA	1:C:304:LEU:HD13	1.92	0.52
1:D:217:CYS:C	1:D:218:GLU:HG3	2.35	0.51
1:D:235:LEU:HD23	1:D:272:MET:HE3	1.91	0.51
1:B:274:ASP:OD1	1:B:300:THR:HG22	2.11	0.51
1:C:79:LEU:HD23	1:C:123:VAL:HG13	1.93	0.51
1:B:126:SER:O	2:B:401:NDP:H6N	2.10	0.50
1:B:257:GLU:H	1:B:257:GLU:CD	2.18	0.50
1:D:217:CYS:O	1:D:218:GLU:CG	2.58	0.50
1:A:154:TRP:O	1:A:155:GLU:CB	2.59	0.50
1:D:340:GLY:O	1:D:341:ARG:CB	2.59	0.50
1:C:129:ALA:HA	1:C:132:PHE:CE1	2.47	0.49
1:D:270:PHE:HE1	1:D:272:MET:CE	2.26	0.49
1:D:300:THR:HG22	1:D:301:HIS:CD2	2.47	0.49
1:B:58:ILE:HG12	2:B:401:NDP:C6A	2.44	0.48
1:C:264:ILE:HG21	1:C:308:LEU:HD21	1.96	0.47
1:C:136:LYS:CB	1:C:142:LEU:HD22	2.14	0.47
1:B:152:ALA:O	1:B:170:LYS:NZ	2.35	0.47
1:D:217:CYS:O	1:D:218:GLU:OE2	2.33	0.46
1:B:270:PHE:CE1	1:B:272:MET:CE	2.88	0.46
1:D:1:MET:O	1:D:1:MET:HG3	2.16	0.46
1:A:93:GLU:HA	1:A:97:LEU:HD12	1.99	0.45
1:C:290:ILE:HB	1:C:291:PRO:HD2	1.98	0.45
1:D:251:VAL:HG13	1:D:255:LYS:HE2	1.99	0.45
1:C:272:MET:HA	1:C:272:MET:HE2	1.99	0.45
1:B:270:PHE:CE1	1:B:272:MET:HE2	2.49	0.44
1:C:218:GLU:OE1	1:C:218:GLU:CA	2.64	0.44
1:D:264:ILE:HG21	1:D:308:LEU:HD21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:CE2	1:B:132:PHE:HB3	2.53	0.43
1:A:240:ILE:HG12	1:A:265:VAL:HG12	1.99	0.43
2:B:401:NDP:H4B	3:B:509:HOH:O	2.19	0.43
1:C:150:ASN:HA	1:C:151:PRO:HD3	1.93	0.43
1:B:57:ASP:CG	1:B:59:SER:HB3	2.44	0.43
1:D:128:TYR:CZ	1:D:132:PHE:HB3	2.54	0.43
1:A:235:LEU:CD2	1:A:272:MET:HE3	2.42	0.43
1:B:146:GLU:OE2	1:B:310:ASN:HA	2.19	0.42
1:B:190:GLU:HG3	1:B:259:ILE:HD12	2.01	0.42
1:C:341:ARG:HA	1:C:341:ARG:HD3	1.76	0.42
1:B:18:ASP:O	1:B:22:LYS:HG3	2.19	0.42
1:A:342:ILE:HG23	1:A:342:ILE:OXT	2.20	0.42
1:C:5:VAL:O	1:C:29:GLY:HA2	2.20	0.42
1:B:302:ASN:HB2	1:B:304:LEU:CD1	2.50	0.42
1:D:153:THR:HA	1:D:171:PHE:HZ	1.85	0.42
1:B:184:ARG:HD2	1:B:184:ARG:HA	1.83	0.41
1:C:310:ASN:HB2	1:C:313:SER:HB2	2.02	0.41
1:A:257:GLU:H	1:A:257:GLU:CD	2.29	0.41
1:B:106:GLY:HA3	3:B:527:HOH:O	2.19	0.41
1:B:264:ILE:HG21	1:B:308:LEU:HD21	2.02	0.41
1:B:223:LEU:HD21	1:B:276:LEU:HG	2.02	0.41
1:C:256:ARG:O	1:C:259:ILE:HG13	2.20	0.41
1:D:198:TYR:OH	1:D:235:LEU:HD11	2.21	0.41
1:A:225:HIS:CE1	1:A:339:GLU:OE2	2.74	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	340/342 (99%)	336 (99%)	2 (1%)	2 (1%)	21 32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	340/342 (99%)	335 (98%)	4 (1%)	1 (0%)	36	50
1	C	300/342 (88%)	292 (97%)	7 (2%)	1 (0%)	36	50
1	D	293/342 (86%)	288 (98%)	4 (1%)	1 (0%)	36	50
All	All	1273/1368 (93%)	1251 (98%)	17 (1%)	5 (0%)	30	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLU
1	C	197	VAL
1	B	197	VAL
1	D	197	VAL
1	A	197	VAL

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	297/297 (100%)	291 (98%)	6 (2%)	48	70
1	B	297/297 (100%)	292 (98%)	5 (2%)	53	74
1	C	265/297 (89%)	248 (94%)	17 (6%)	16	28
1	D	263/297 (89%)	253 (96%)	10 (4%)	29	49
All	All	1122/1188 (94%)	1084 (97%)	38 (3%)	32	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	83	SER
1	A	117	ASP
1	A	132	PHE
1	A	184	ARG
1	A	223	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	19	LEU
1	B	118	SER
1	B	123	VAL
1	B	132	PHE
1	B	289	ASN
1	C	2	SER
1	C	24	ASP
1	C	58	ILE
1	C	123	VAL
1	C	132	PHE
1	C	137	GLU
1	C	143	THR
1	C	184	ARG
1	C	222	SER
1	C	230	ASP
1	C	256	ARG
1	C	259	ILE
1	C	285	VAL
1	C	292	VAL
1	C	320	LYS
1	C	333	SER
1	C	341	ARG
1	D	73	LYS
1	D	81	THR
1	D	105	LYS
1	D	132	PHE
1	D	137	GLU
1	D	218	GLU
1	D	257	GLU
1	D	261	GLN
1	D	285	VAL
1	D	300	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	301	HIS
1	B	221	ASN
1	B	289	ASN
1	C	109	HIS
1	C	203	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	34	GLN
1	D	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	NDP	B	401	-	51,52,52	1.49	9 (17%)	71,80,80	1.55	9 (12%)
2	NDP	A	401	-	51,52,52	1.49	3 (5%)	71,80,80	1.60	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	NDP	B	401	-	-	9/34/77/77	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	401	-	-	10/34/77/77	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NDP	O7N-C7N	7.52	1.42	1.24
2	B	401	NDP	O7N-C7N	7.13	1.41	1.24
2	B	401	NDP	C2A-N1A	2.68	1.38	1.33
2	B	401	NDP	C2A-N3A	2.67	1.38	1.33
2	A	401	NDP	C2A-N1A	2.64	1.38	1.33
2	A	401	NDP	C2A-N3A	2.60	1.38	1.33
2	B	401	NDP	C8A-N7A	2.34	1.36	1.31
2	B	401	NDP	PN-O3	2.21	1.61	1.59
2	B	401	NDP	PA-O3	2.16	1.61	1.59
2	B	401	NDP	C5A-N7A	-2.14	1.35	1.39
2	B	401	NDP	C6N-C5N	2.04	1.39	1.33
2	B	401	NDP	C2N-C3N	2.01	1.40	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NDP	N3A-C2A-N1A	-6.14	119.29	128.58
2	B	401	NDP	N3A-C2A-N1A	-5.69	119.97	128.58
2	A	401	NDP	N9A-C8A-N7A	-4.46	107.60	113.94
2	B	401	NDP	C5A-C4A-N3A	-4.27	120.84	126.72
2	A	401	NDP	C5A-C4A-N3A	-3.97	121.25	126.72
2	B	401	NDP	N9A-C8A-N7A	-3.93	108.36	113.94
2	A	401	NDP	C5A-N7A-C8A	3.55	109.03	103.45
2	B	401	NDP	C5A-N7A-C8A	3.51	108.97	103.45
2	A	401	NDP	C2A-N3A-C4A	3.44	120.23	111.83
2	B	401	NDP	C2A-N3A-C4A	3.39	120.12	111.83
2	B	401	NDP	O4D-C1D-N1N	3.07	113.93	108.08
2	A	401	NDP	O4D-C1D-N1N	2.82	113.46	108.08
2	A	401	NDP	N3A-C4A-N9A	2.81	131.94	127.17
2	A	401	NDP	C4A-N9A-C8A	2.78	108.66	105.74
2	B	401	NDP	C4A-C5A-N7A	-2.70	107.50	110.58
2	B	401	NDP	C1D-N1N-C6N	-2.67	115.12	120.77
2	A	401	NDP	C6N-N1N-C2N	2.61	122.11	119.32
2	A	401	NDP	C1D-N1N-C6N	-2.57	115.35	120.77
2	B	401	NDP	N3A-C4A-N9A	2.43	131.31	127.17
2	A	401	NDP	C4A-C5A-N7A	-2.35	107.89	110.58

There are no chirality outliers.

All (19) torsion outliers are listed below:

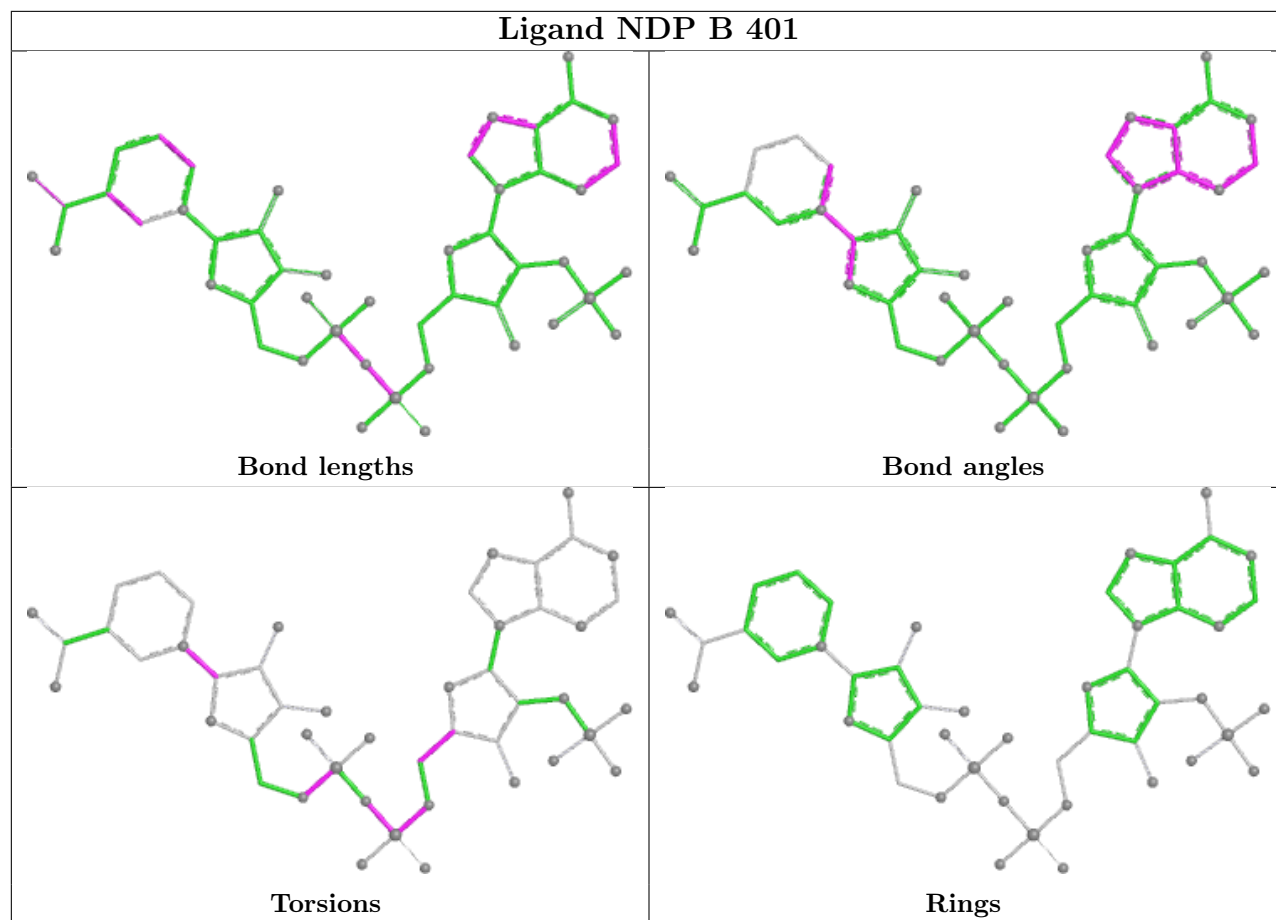
Mol	Chain	Res	Type	Atoms
2	A	401	NDP	C5B-O5B-PA-O1A
2	A	401	NDP	C5B-O5B-PA-O2A
2	A	401	NDP	C5B-O5B-PA-O3
2	A	401	NDP	C5D-O5D-PN-O3
2	A	401	NDP	C5D-O5D-PN-O1N
2	B	401	NDP	C5B-O5B-PA-O1A
2	B	401	NDP	C5B-O5B-PA-O2A
2	B	401	NDP	C5B-O5B-PA-O3
2	B	401	NDP	PN-O3-PA-O5B
2	B	401	NDP	C5D-O5D-PN-O3
2	B	401	NDP	C5D-O5D-PN-O1N
2	A	401	NDP	O4D-C1D-N1N-C6N
2	A	401	NDP	PN-O3-PA-O5B
2	B	401	NDP	O4D-C1D-N1N-C6N
2	A	401	NDP	C5D-O5D-PN-O2N
2	B	401	NDP	C5D-O5D-PN-O2N
2	A	401	NDP	O4B-C4B-C5B-O5B
2	B	401	NDP	O4B-C4B-C5B-O5B
2	A	401	NDP	C3B-C2B-O2B-P2B

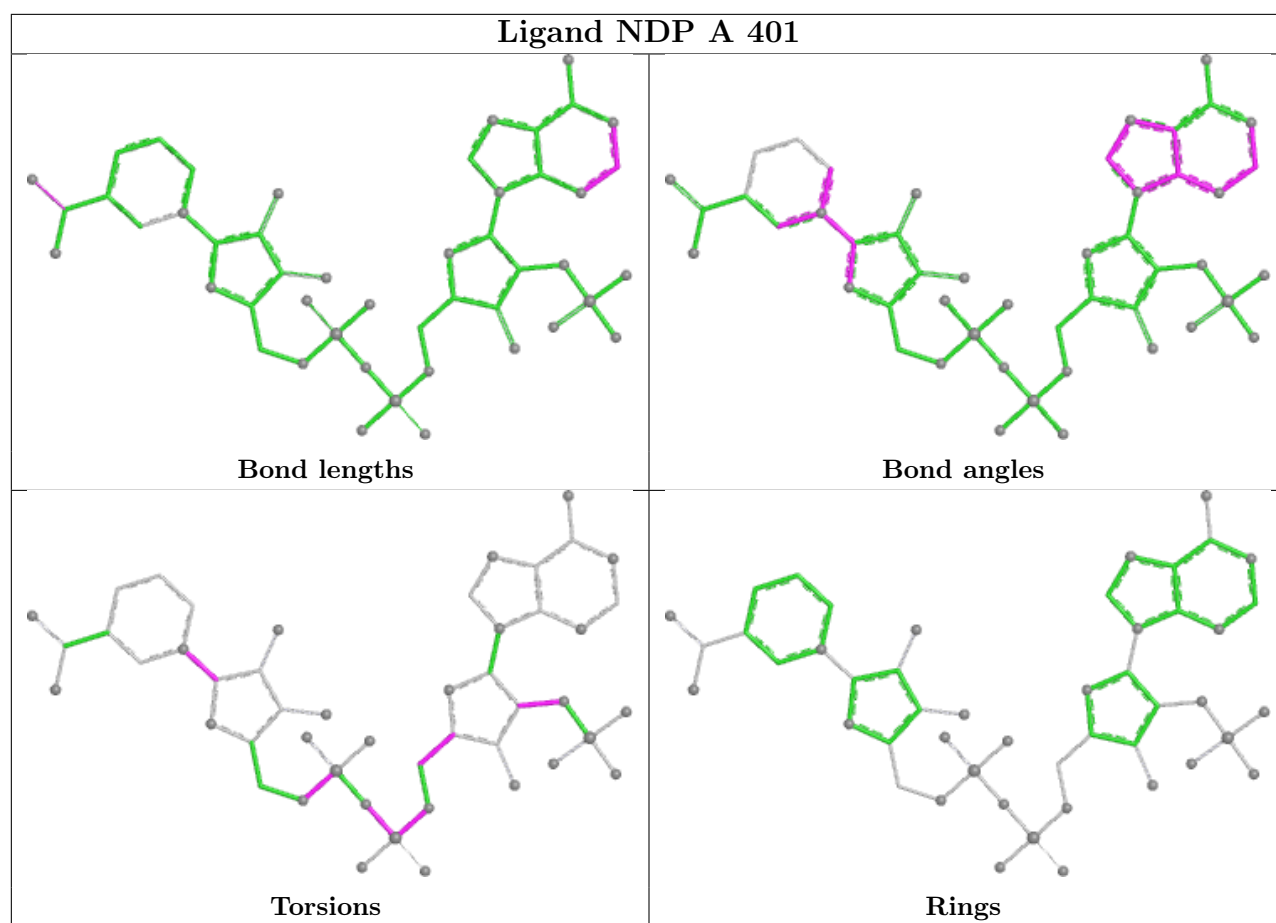
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NDP	3	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	342/342 (100%)	0.33	13 (3%) 44 40	26, 44, 69, 90	0
1	B	342/342 (100%)	0.52	15 (4%) 39 34	26, 49, 77, 95	0
1	C	308/342 (90%)	0.51	24 (7%) 19 15	28, 47, 96, 109	0
1	D	305/342 (89%)	0.74	47 (15%) 5 4	28, 50, 86, 131	0
All	All	1297/1368 (94%)	0.52	99 (7%) 20 16	26, 48, 78, 131	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	143	THR	5.7
1	D	131	VAL	5.7
1	C	82	ALA	5.5
1	D	128	TYR	5.2
1	D	307	THR	5.1
1	D	145	ASN	5.0
1	D	97	LEU	4.4
1	D	340	GLY	4.3
1	C	135	ALA	4.3
1	D	133	ASP	4.1
1	D	168	SER	4.0
1	C	1	MET	3.9
1	D	153	THR	3.8
1	D	171	PHE	3.7
1	D	152	ALA	3.5
1	D	84	PRO	3.5
1	D	151	PRO	3.4
1	C	151	PRO	3.4
1	C	97	LEU	3.3
1	D	1	MET	3.2
1	D	211	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	143	THR	3.2
1	B	132	PHE	3.1
1	D	302	ASN	3.1
1	C	171	PHE	3.0
1	C	117	ASP	2.9
1	D	338	PHE	2.9
1	D	98	ILE	2.8
1	B	252	ALA	2.8
1	B	300	THR	2.8
1	D	140	LYS	2.8
1	B	135	ALA	2.7
1	D	195	ASN	2.7
1	C	153	THR	2.7
1	B	88	ASP	2.7
1	C	140	LYS	2.7
1	C	148	SER	2.7
1	B	1	MET	2.6
1	D	130	ALA	2.6
1	C	81	THR	2.6
1	D	82	ALA	2.6
1	A	1	MET	2.5
1	D	67	VAL	2.5
1	D	144	PHE	2.5
1	C	149	TRP	2.5
1	D	138	ASN	2.5
1	C	303	THR	2.5
1	D	132	PHE	2.4
1	C	289	ASN	2.4
1	D	303	THR	2.4
1	A	88	ASP	2.4
1	B	342	ILE	2.4
1	C	74	ASP	2.4
1	A	207	LYS	2.4
1	D	339	GLU	2.4
1	C	236	PHE	2.4
1	D	129	ALA	2.4
1	A	338	PHE	2.3
1	D	137	GLU	2.3
1	B	134	MET	2.3
1	B	285	VAL	2.3
1	D	81	THR	2.3
1	D	99	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	83	SER	2.3
1	A	117	ASP	2.3
1	D	236	PHE	2.3
1	D	308	LEU	2.2
1	C	218	GLU	2.2
1	D	341	ARG	2.2
1	D	141	SER	2.2
1	A	336	LEU	2.2
1	B	155	GLU	2.2
1	B	181	GLU	2.2
1	C	150	ASN	2.2
1	D	150	ASN	2.2
1	C	84	PRO	2.2
1	A	131	VAL	2.1
1	A	342	ILE	2.1
1	A	186	SER	2.1
1	D	117	ASP	2.1
1	A	66	HIS	2.1
1	B	138	ASN	2.1
1	C	302	ASN	2.1
1	D	183	ASN	2.1
1	D	217	CYS	2.1
1	C	99	PRO	2.1
1	D	326	GLU	2.1
1	D	83	SER	2.1
1	A	233	PRO	2.1
1	A	226	LEU	2.0
1	D	218	GLU	2.0
1	D	74	ASP	2.0
1	C	129	ALA	2.0
1	A	339	GLU	2.0
1	D	96	LEU	2.0
1	B	140	LYS	2.0
1	B	185	ASP	2.0
1	B	186	SER	2.0
1	D	59	SER	2.0

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

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

6.3 Carbohydrates [i](#)

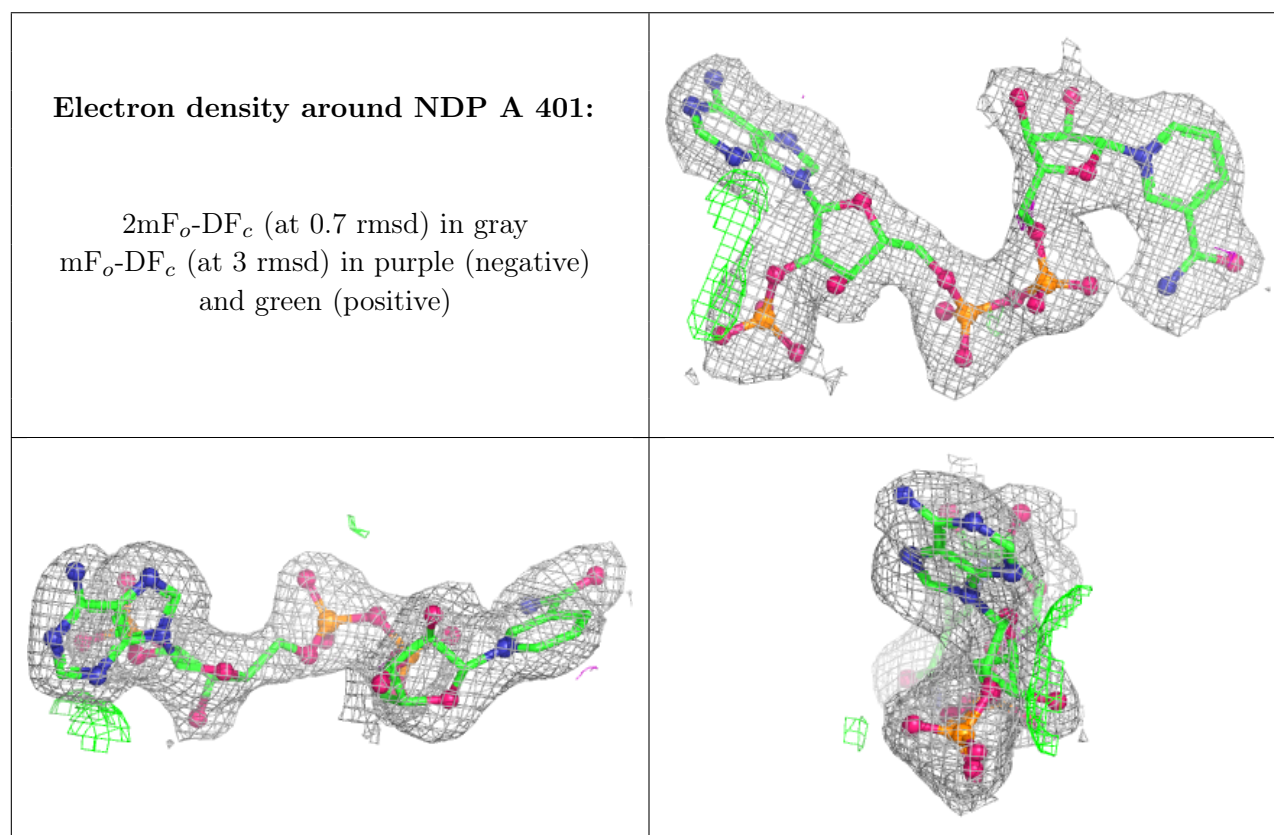
There are no oligosaccharides in this entry.

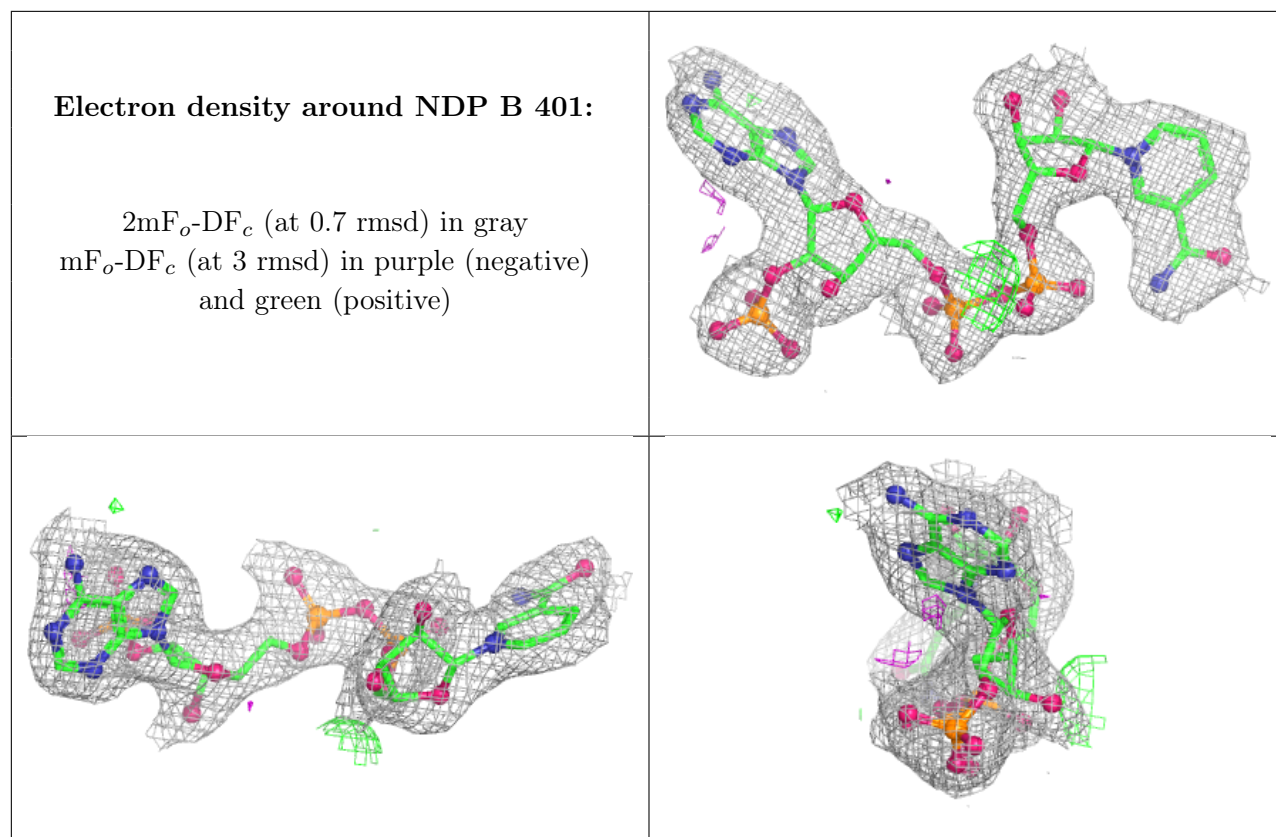
6.4 Ligands [i](#)

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	NDP	A	401	48/48	0.95	0.08	34,38,41,42	0
2	NDP	B	401	48/48	0.95	0.08	34,36,39,41	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.