



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2026 – 04:15 pm BST

PDB ID : 9QWY / pdb_00009qwy
Title : Crystal structure of an NtA622L variant in complex with NADPH and Trigonelline
Authors : Mokos, D.; Leitner, D.; Daniel, B.
Deposited on : 2025-04-15
Resolution : 2.60 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	:	1.8.4, CSD as541be (2020)
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

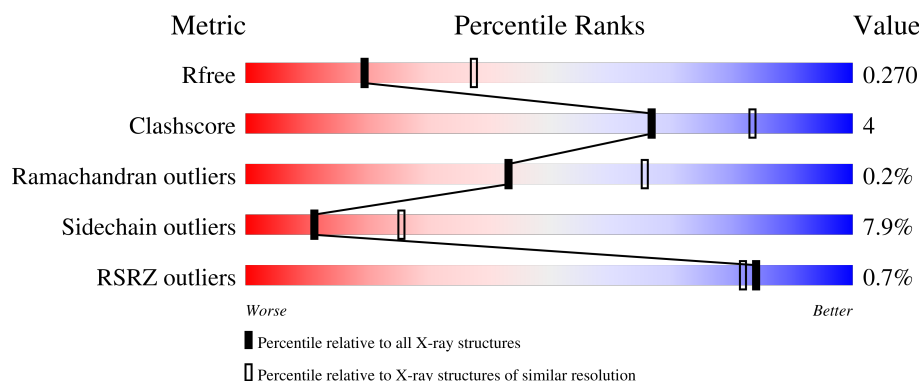
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	310	 77% 17% 2% 4%
1	B	310	 79% 17% 2% 4%
1	C	310	 2% 78% 16% 5% 1%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14997 atoms, of which 7467 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.

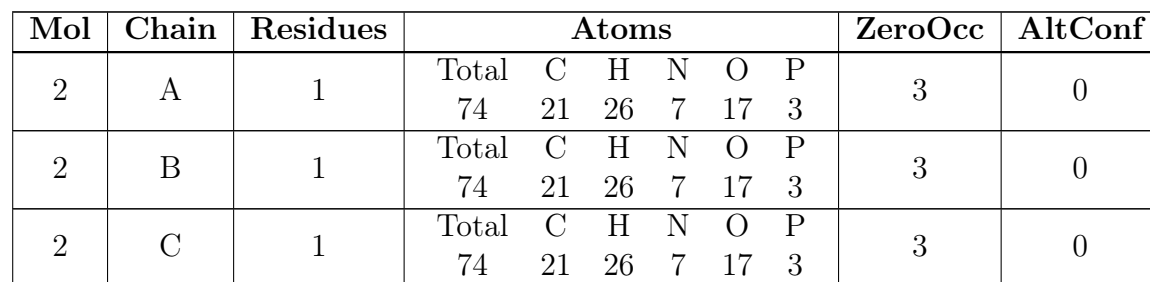
- Molecule 1 is a protein called Isoflavone reductase homolog A622-like.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	H	N	O	S	61	0	0
			4873	1566	2456	392	455	4			
1	B	306	Total	C	H	N	O	S	61	0	0
			4873	1566	2456	392	455	4			
1	C	306	Total	C	H	N	O	S	61	0	0
			4873	1566	2456	392	455	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ASN	LYS	engineered mutation	UNP B6VRE6
A	201	ILE	MET	engineered mutation	UNP B6VRE6
A	259	LEU	MET	engineered mutation	UNP B6VRE6
B	99	ASN	LYS	engineered mutation	UNP B6VRE6
B	201	ILE	MET	engineered mutation	UNP B6VRE6
B	259	LEU	MET	engineered mutation	UNP B6VRE6
C	99	ASN	LYS	engineered mutation	UNP B6VRE6
C	201	ILE	MET	engineered mutation	UNP B6VRE6
C	259	LEU	MET	engineered mutation	UNP B6VRE6

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



- A1JBP
-
- Chemical structure of A1JBP (4-(pyridinium-2-yl)acetic acid). The structure shows a pyridinium ring with a positive charge on the nitrogen atom (N1). The ring carbons are labeled C2 through C6. A carboxylic acid group is attached to C2, with the carbonyl carbon labeled C1, the carbonyl oxygen labeled O1, and the hydroxyl oxygen labeled O2. A methyl group (C7) is attached to N1. The structure is drawn with blue lines for the pyridinium ring and red lines for the carboxylic acid group.

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

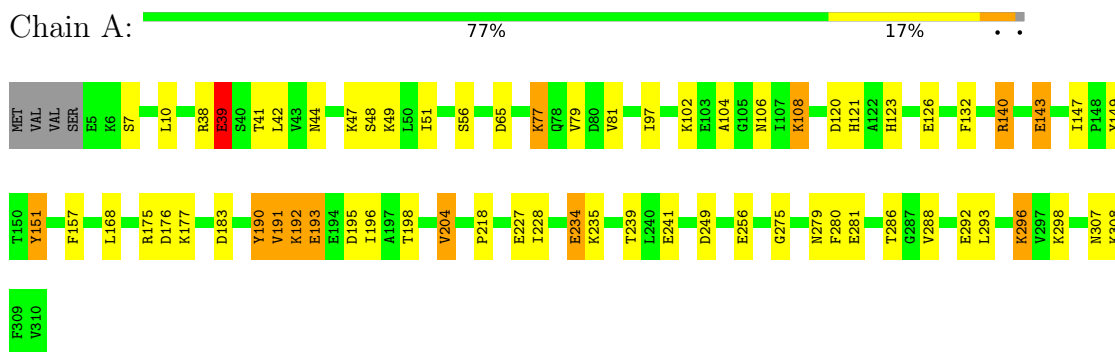
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	33	Total	O	0	0
			33	33		
4	C	33	Total	O	0	0
			33	33		

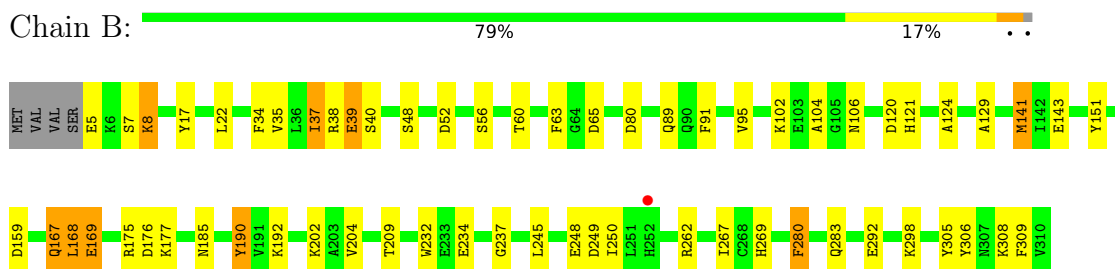
3 Residue-property plots [i](#)

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.

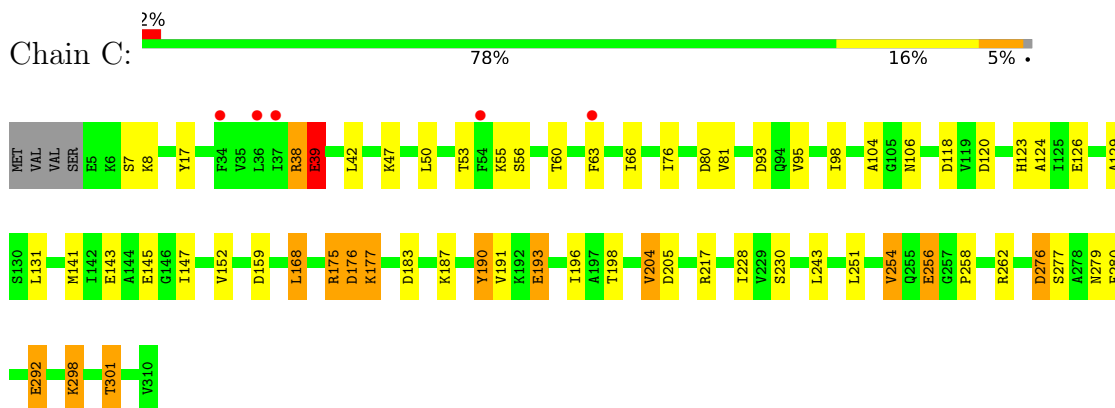
- Molecule 1: Isoflavone reductase homolog A622-like



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.23Å 64.92Å 115.35Å 90.00° 101.51° 90.00°	Depositor
Resolution (Å)	56.29 – 2.60 56.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (56.29-2.60) 97.6 (56.29-2.60)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.206 , 0.268 0.208 , 0.270	Depositor DCC
R_{free} test set	1471 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14997	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: NDP, A1JBP

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	1.05	2/2470 (0.1%)	1.66	36/3351 (1.1%)
1	B	0.96	1/2470 (0.0%)	1.61	30/3351 (0.9%)
1	C	0.95	0/2470	1.60	30/3351 (0.9%)
All	All	0.99	3/7410 (0.0%)	1.62	96/10053 (1.0%)

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	1
1	B	0	3
1	C	0	5
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	SER	CA-CB	-5.76	1.44	1.53
1	A	56	SER	C-O	-5.15	1.17	1.24
1	A	123	HIS	CE1-NE2	5.01	1.37	1.32

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	GLU	CB-CG-CD	9.02	127.94	112.60
1	B	167	GLN	CB-CA-C	8.83	125.87	110.85
1	A	120	ASP	CA-CB-CG	8.61	121.21	112.60
1	C	292	GLU	N-CA-CB	7.90	121.73	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ASP	CA-CB-CG	7.71	120.31	112.60
1	C	176	ASP	CA-CB-CG	7.58	120.18	112.60
1	B	176	ASP	CA-CB-CG	7.37	119.97	112.60
1	C	187	LYS	CB-CG-CD	7.13	127.70	111.30
1	C	123	HIS	CA-CB-CG	-7.10	106.70	113.80
1	A	176	ASP	CA-CB-CG	7.00	119.60	112.60
1	B	209	THR	OG1-CB-CG2	6.96	123.21	109.30
1	A	193	GLU	CB-CG-CD	6.84	124.22	112.60
1	A	143	GLU	CG-CD-OE2	-6.77	102.82	118.40
1	B	292	GLU	CB-CG-CD	6.56	123.76	112.60
1	A	286	THR	CA-C-N	6.47	126.05	121.65
1	A	286	THR	C-N-CA	6.47	126.05	121.65
1	B	120	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	292	GLU	N-CA-CB	6.38	119.26	110.01
1	A	108	LYS	CB-CA-C	6.37	120.26	109.55
1	A	140	ARG	CD-NE-CZ	6.32	133.24	124.40
1	A	256	GLU	N-CA-CB	-6.23	99.98	110.83
1	B	63	PHE	CB-CA-C	6.23	120.03	109.75
1	B	38	ARG	CB-CA-C	-6.18	99.75	110.45
1	A	151	TYR	CA-C-N	-6.16	114.68	122.37
1	A	151	TYR	C-N-CA	-6.16	114.68	122.37
1	C	301	THR	CA-CB-OG1	-6.15	100.37	109.60
1	B	91	PHE	N-CA-CB	6.15	119.16	110.12
1	B	168	LEU	N-CA-CB	6.14	120.88	110.49
1	B	245	LEU	N-CA-CB	-6.11	100.99	110.65
1	B	80	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	248	GLU	CB-CG-CD	6.08	122.93	112.60
1	B	39	GLU	CB-CG-CD	6.06	122.91	112.60
1	A	296	LYS	CG-CD-CE	6.04	125.20	111.30
1	A	183	ASP	CA-CB-CG	6.04	118.64	112.60
1	C	280	PHE	CA-CB-CG	6.01	119.81	113.80
1	C	175	ARG	N-CA-CB	-6.00	102.32	110.95
1	B	143	GLU	CB-CA-C	5.96	120.24	110.88
1	A	143	GLU	CG-CD-OE1	5.96	132.10	118.40
1	C	63	PHE	CB-CA-C	5.94	119.56	109.75
1	A	157	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	234	GLU	CB-CG-CD	5.88	122.60	112.60
1	C	126	GLU	CB-CG-CD	5.87	122.57	112.60
1	A	234	GLU	N-CA-CB	5.82	118.67	110.12
1	A	191	VAL	N-CA-CB	5.82	120.98	111.44
1	C	143	GLU	CB-CA-C	5.82	120.01	110.88
1	C	93	ASP	CA-CB-CG	5.81	118.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ASP	CB-CA-C	-5.79	99.83	109.55
1	C	38	ARG	CB-CA-C	-5.78	100.05	111.60
1	C	183	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	120	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	256	GLU	CB-CA-C	5.72	120.29	109.37
1	B	8	LYS	CB-CG-CD	5.70	124.40	111.30
1	A	298	LYS	CB-CA-C	5.69	120.80	111.41
1	B	141	MET	CG-SD-CE	-5.68	88.39	100.90
1	A	198	THR	N-CA-CB	5.66	118.17	109.91
1	B	280	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	249	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	126	GLU	CB-CG-CD	5.60	122.12	112.60
1	C	230	SER	CA-C-N	5.60	128.10	120.54
1	C	230	SER	C-N-CA	5.60	128.10	120.54
1	C	80	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	65	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	169	GLU	CB-CA-C	5.49	120.26	109.72
1	C	17	TYR	O-C-N	5.46	127.69	122.07
1	C	143	GLU	CG-CD-OE1	5.46	130.96	118.40
1	B	65	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	39	GLU	CG-CD-OE2	5.40	130.82	118.40
1	B	5	GLU	CB-CA-C	5.38	120.32	110.10
1	A	280	PHE	CA-CB-CG	5.37	119.17	113.80
1	B	151	TYR	CA-C-N	-5.37	115.66	122.37
1	B	151	TYR	C-N-CA	-5.37	115.66	122.37
1	B	234	GLU	CB-CA-C	5.35	119.66	110.79
1	C	118	ASP	N-CA-CB	5.34	117.99	110.24
1	A	249	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	132	PHE	CA-C-O	-5.28	114.95	120.55
1	C	177	LYS	N-CA-CB	-5.26	101.90	110.59
1	A	296	LYS	CB-CA-C	5.23	119.77	109.72
1	A	97	ILE	O-C-N	5.23	127.03	121.91
1	B	63	PHE	N-CA-CB	-5.20	101.95	110.43
1	A	77	LYS	CB-CG-CD	5.19	123.24	111.30
1	A	192	LYS	CB-CA-C	5.15	118.46	109.65
1	C	8	LYS	CB-CG-CD	5.13	123.10	111.30
1	C	145	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	227	GLU	CG-CD-OE1	-5.11	106.64	118.40
1	B	102	LYS	CB-CA-C	-5.11	102.63	110.81
1	C	258	PRO	N-CA-C	-5.10	103.81	111.57
1	A	195	ASP	O-C-N	5.09	127.51	122.12
1	C	60	THR	CA-CB-OG1	-5.08	101.99	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	THR	CA-CB-OG1	5.08	117.22	109.60
1	C	193	GLU	CB-CG-CD	5.07	121.21	112.60
1	B	17	TYR	CA-C-N	5.02	128.61	120.82
1	B	17	TYR	C-N-CA	5.02	128.61	120.82
1	A	149	TYR	OH-CZ-CE2	5.02	134.96	119.90
1	A	143	GLU	CB-CA-C	5.01	118.75	110.88
1	B	185	ASN	CB-CA-C	-5.01	100.30	110.17
1	A	296	LYS	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ARG	Sidechain
1	B	175	ARG	Sidechain
1	B	237	GLY	Peptide
1	B	262	ARG	Sidechain
1	C	175	ARG	Sidechain
1	C	176	ASP	Peptide
1	C	217	ARG	Sidechain
1	C	262	ARG	Sidechain
1	C	38	ARG	Sidechain

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	2417	2456	2449	17	1
1	B	2417	2456	2449	17	1
1	C	2417	2456	2449	20	0
2	A	48	26	26	1	0
2	B	48	26	26	0	0
2	C	48	26	25	2	0
3	A	10	7	0	0	0
3	B	10	7	0	0	0
3	C	10	7	0	0	0
4	A	39	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	33	0	0	7	0
4	C	33	0	0	6	0
All	All	7530	7467	7424	55	1

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 (55) 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:50:LEU:HA	4:C:501:HOH:O	1.78	0.82
1:A:121:HIS:HB3	4:A:532:HOH:O	1.80	0.81
1:B:309:PHE:HB2	4:B:501:HOH:O	1.82	0.79
1:B:306:TYR:O	4:B:501:HOH:O	2.02	0.76
2:A:401:NDP:H8A	4:A:511:HOH:O	1.88	0.72
1:C:66:ILE:HG22	2:C:401:NDP:N6A	2.05	0.70
1:B:35:VAL:HG12	1:B:37:ILE:HD13	1.79	0.64
1:B:35:VAL:HG12	1:B:37:ILE:CD1	2.29	0.62
1:C:298:LYS:HA	4:C:520:HOH:O	2.01	0.61
1:B:167:GLN:C	4:B:505:HOH:O	2.43	0.60
1:A:44:ASN:OD1	1:A:47:LYS:HG2	2.01	0.59
1:C:66:ILE:HG22	2:C:401:NDP:H62A	1.72	0.55
1:C:76:ILE:HG21	4:C:512:HOH:O	2.07	0.54
1:B:167:GLN:HB2	4:B:505:HOH:O	2.07	0.53
1:B:167:GLN:CB	4:B:505:HOH:O	2.56	0.52
1:C:104:ALA:HB1	1:C:106:ASN:OD1	2.10	0.52
1:A:140:ARG:NH1	1:A:143:GLU:OE2	2.44	0.50
1:B:104:ALA:HB1	1:B:106:ASN:OD1	2.12	0.50
1:C:276:ASP:HA	1:C:279:ASN:OD1	2.12	0.49
1:A:81:VAL:HG21	1:A:204:VAL:HG13	1.96	0.48
1:B:305:TYR:O	1:B:308:LYS:CE	2.62	0.47
1:B:305:TYR:O	1:B:308:LYS:HE2	2.14	0.47
1:C:81:VAL:HG21	1:C:204:VAL:HG13	1.97	0.47
1:A:104:ALA:HB1	1:A:106:ASN:OD1	2.15	0.47
1:A:288:VAL:CG2	1:A:293:LEU:HD11	2.45	0.46
1:B:190:TYR:CD1	1:B:190:TYR:N	2.83	0.46
1:C:190:TYR:CD1	1:C:190:TYR:N	2.83	0.46
1:C:76:ILE:HD13	4:C:512:HOH:O	2.15	0.46
1:B:168:LEU:N	4:B:505:HOH:O	2.47	0.46
1:A:190:TYR:N	1:A:190:TYR:CD1	2.84	0.45
1:B:121:HIS:CD2	1:B:280:PHE:CD1	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HB2	1:A:79:VAL:HG11	1.98	0.44
1:A:191:VAL:HG12	1:A:218:PRO:HG2	2.00	0.44
1:B:124:ALA:O	1:B:129:ALA:HB2	2.18	0.43
1:B:232:TRP:HZ3	4:B:501:HOH:O	2.00	0.43
1:A:38:ARG:O	1:A:41:THR:N	2.52	0.43
1:C:251:LEU:O	1:C:254:VAL:HG12	2.19	0.43
1:A:193:GLU:HA	1:A:196:ILE:HD12	2.01	0.42
1:A:275:GLY:O	1:A:279:ASN:CG	2.62	0.42
1:B:250:ILE:HG21	1:B:269:HIS:HB2	2.01	0.42
1:C:193:GLU:HB2	4:C:503:HOH:O	2.18	0.42
1:B:34:PHE:CD2	1:B:60:THR:HB	2.55	0.42
1:A:288:VAL:HG21	1:A:293:LEU:HD11	2.02	0.41
1:C:124:ALA:O	1:C:129:ALA:HB2	2.20	0.41
1:C:39:GLU:O	1:C:39:GLU:CD	2.64	0.41
1:C:191:VAL:HG12	1:C:196:ILE:HG13	2.02	0.41
1:C:256:GLU:OE2	1:C:256:GLU:HA	2.20	0.41
1:C:95:VAL:HG22	1:C:141:MET:SD	2.61	0.41
1:C:152:VAL:HG23	4:C:508:HOH:O	2.20	0.41
1:A:81:VAL:HG11	1:A:204:VAL:CG1	2.51	0.40
1:A:151:TYR:HA	4:A:508:HOH:O	2.21	0.40
1:A:41:THR:HG22	1:A:51:ILE:HD11	2.03	0.40
1:C:98:ILE:HG21	1:C:141:MET:HG2	2.02	0.40
1:A:235:LYS:NZ	1:A:307:ASN:OD1	2.54	0.40
1:C:98:ILE:HG23	1:C:147:ILE:HD12	2.03	0.40

All (1) 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:39:GLU:OE1	1:B:167:GLN:NE2[2_655]	2.18	0.02

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	304/310 (98%)	293 (96%)	10 (3%)	1 (0%)	36	58
1	B	304/310 (98%)	292 (96%)	12 (4%)	0	100	100
1	C	304/310 (98%)	294 (97%)	9 (3%)	1 (0%)	36	58
All	All	912/930 (98%)	879 (96%)	31 (3%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	LEU
1	C	168	LEU

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	267/271 (98%)	246 (92%)	21 (8%)	11	26
1	B	267/271 (98%)	246 (92%)	21 (8%)	11	26
1	C	267/271 (98%)	246 (92%)	21 (8%)	11	26
All	All	801/813 (98%)	738 (92%)	63 (8%)	11	26

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	39	GLU
1	A	42	LEU
1	A	48	SER
1	A	49	LYS
1	A	77	LYS
1	A	102	LYS
1	A	108	LYS
1	A	147	ILE

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Mol	Chain	Res	Type
1	A	177	LYS
1	A	190	TYR
1	A	192	LYS
1	A	204	VAL
1	A	228	ILE
1	A	234	GLU
1	A	239	THR
1	A	241	GLU
1	A	281	GLU
1	A	292	GLU
1	A	296	LYS
1	A	308	LYS
1	B	7	SER
1	B	8	LYS
1	B	22	LEU
1	B	37	ILE
1	B	39	GLU
1	B	48	SER
1	B	52	ASP
1	B	56	SER
1	B	89	GLN
1	B	95	VAL
1	B	141	MET
1	B	159	ASP
1	B	169	GLU
1	B	177	LYS
1	B	190	TYR
1	B	192	LYS
1	B	202	LYS
1	B	204	VAL
1	B	267	ILE
1	B	283	GLN
1	B	298	LYS
1	C	7	SER
1	C	39	GLU
1	C	42	LEU
1	C	47	LYS
1	C	53	THR
1	C	55	LYS
1	C	56	SER
1	C	131	LEU
1	C	159	ASP

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Mol	Chain	Res	Type
1	C	168	LEU
1	C	177	LYS
1	C	190	TYR
1	C	204	VAL
1	C	228	ILE
1	C	243	LEU
1	C	254	VAL
1	C	256	GLU
1	C	277	SER
1	C	292	GLU
1	C	298	LYS
1	C	301	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	123	HIS
1	B	44	ASN
1	B	90	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](#)

6 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	A	401	-	49,52,52	1.08	3 (6%)	66,80,80	1.95	19 (28%)
2	NDP	C	401	-	49,52,52	0.92	1 (2%)	66,80,80	2.02	16 (24%)
3	A1JBP	A	402	-	10,10,10	0.83	0	13,13,13	0.83	0
3	A1JBP	C	402	-	10,10,10	1.24	2 (20%)	13,13,13	0.69	0
2	NDP	B	401	-	49,52,52	0.89	2 (4%)	66,80,80	1.36	8 (12%)
3	A1JBP	B	402	-	10,10,10	1.07	1 (10%)	13,13,13	1.41	3 (23%)

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	A	401	-	-	10/34/77/77	0/5/5/5
2	NDP	C	401	-	-	15/34/77/77	0/5/5/5
3	A1JBP	A	402	-	-	4/4/4/4	0/1/1/1
3	A1JBP	C	402	-	-	4/4/4/4	0/1/1/1
2	NDP	B	401	-	-	16/34/77/77	0/5/5/5
3	A1JBP	B	402	-	-	4/4/4/4	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NDP	P2B-O2B	3.68	1.66	1.59
2	B	401	NDP	P2B-O2B	3.44	1.65	1.59
2	A	401	NDP	C8A-N9A	2.75	1.42	1.37
3	C	402	A1JBP	O1-C1	2.57	1.30	1.22
2	A	401	NDP	P2B-O3X	-2.43	1.45	1.54
2	A	401	NDP	C6N-C5N	-2.40	1.29	1.33
3	C	402	A1JBP	C2-C1	2.23	1.54	1.49
2	B	401	NDP	C1D-N1N	2.20	1.52	1.46
3	B	402	A1JBP	O1-C1	2.04	1.28	1.22

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NDP	O3B-C3B-C2B	8.13	134.26	111.17
2	A	401	NDP	O4B-C1B-C2B	-5.96	96.11	106.57
2	A	401	NDP	C2B-C1B-N9A	5.83	123.35	113.53
2	C	401	NDP	C2B-C3B-C4B	-4.44	92.35	101.99
2	C	401	NDP	O2B-C2B-C3B	4.41	127.66	111.68
2	A	401	NDP	O3B-C3B-C4B	-3.95	99.62	111.05
2	A	401	NDP	C5A-N7A-C8A	-3.83	98.06	103.51
2	B	401	NDP	PN-O3-PA	-3.77	119.88	132.83
2	C	401	NDP	O2B-C2B-C1B	-3.76	96.57	110.10
2	C	401	NDP	O4B-C4B-C3B	-3.71	97.77	105.11
2	C	401	NDP	O4B-C1B-N9A	3.64	115.24	108.06
2	B	401	NDP	O2D-C2D-C3D	3.44	122.94	111.82
2	A	401	NDP	C1D-N1N-C2N	-3.36	115.52	121.11
2	A	401	NDP	O3B-C3B-C2B	3.30	120.54	111.17
2	C	401	NDP	O4B-C4B-C5B	3.25	120.08	109.37
2	A	401	NDP	C4A-C5A-N7A	3.25	114.58	110.62
2	C	401	NDP	O3X-P2B-O2B	3.24	120.50	105.99
2	A	401	NDP	N9A-C8A-N7A	3.22	118.32	113.91
2	B	401	NDP	C1D-N1N-C2N	-3.11	115.94	121.11
2	C	401	NDP	C4A-N9A-C1B	3.04	133.83	126.59
2	B	401	NDP	O2A-PA-O1A	-3.03	97.27	112.24
3	B	402	A1JBP	O1-C1-C2	-2.92	113.66	121.45
2	C	401	NDP	C3B-C2B-C1B	-2.87	97.50	102.89
2	A	401	NDP	O2B-C2B-C1B	2.83	120.29	110.10
2	C	401	NDP	O3D-C3D-C4D	2.75	118.99	111.05
2	A	401	NDP	O4B-C1B-N9A	2.71	113.40	108.06
2	A	401	NDP	C4A-N9A-C8A	-2.68	102.83	105.73
2	A	401	NDP	C5A-C4A-N3A	2.65	130.21	126.75
2	C	401	NDP	C1B-N9A-C8A	-2.64	121.16	127.14
2	C	401	NDP	O2X-P2B-O2B	-2.58	94.45	105.99
2	B	401	NDP	O4D-C1D-N1N	2.52	112.98	108.06
2	A	401	NDP	C3B-C2B-C1B	-2.52	98.16	102.89
2	A	401	NDP	C3N-C7N-N7N	-2.50	113.23	117.67
2	B	401	NDP	C3D-C2D-C1D	-2.46	96.76	101.43
2	B	401	NDP	O5B-PA-O1A	-2.45	99.51	109.07
2	B	401	NDP	C3B-C2B-C1B	-2.44	98.29	102.89
2	A	401	NDP	O2B-C2B-C3B	-2.40	102.99	111.68
2	A	401	NDP	PN-O3-PA	-2.36	124.74	132.83
3	B	402	A1JBP	O2-C1-O1	2.28	128.40	123.35
2	A	401	NDP	C1B-N9A-C8A	2.15	132.00	127.14
2	C	401	NDP	PA-O5B-C5B	2.15	134.30	121.68
3	B	402	A1JBP	C6-C2-C3	2.15	120.69	118.26
2	C	401	NDP	C2D-C3D-C4D	-2.13	98.50	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NDP	C6A-C5A-N7A	-2.11	128.08	132.02
2	A	401	NDP	N3A-C4A-N9A	-2.11	123.61	127.08
2	A	401	NDP	O3X-P2B-O2X	2.07	115.54	107.64

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NDP	C5D-O5D-PN-O1N
2	B	401	NDP	C5D-O5D-PN-O3
2	C	401	NDP	C5B-O5B-PA-O1A
2	C	401	NDP	C5B-O5B-PA-O3
2	C	401	NDP	O4B-C4B-C5B-O5B
2	C	401	NDP	C2B-C1B-N9A-C4A
2	C	401	NDP	C2B-C1B-N9A-C8A
2	A	401	NDP	C2D-C1D-N1N-C2N
2	C	401	NDP	C3B-C4B-C5B-O5B
2	B	401	NDP	C1B-C2B-O2B-P2B
2	B	401	NDP	C3B-C2B-O2B-P2B
3	B	402	A1JBP	O1-C1-C2-C3
2	A	401	NDP	C2D-C1D-N1N-C6N
3	C	402	A1JBP	O2-C1-C2-C3
3	C	402	A1JBP	O1-C1-C2-C3
2	C	401	NDP	C3B-C2B-O2B-P2B
3	B	402	A1JBP	O2-C1-C2-C3
3	A	402	A1JBP	O1-C1-C2-C3
3	C	402	A1JBP	O1-C1-C2-C6
3	C	402	A1JBP	O2-C1-C2-C6
2	B	401	NDP	O4D-C4D-C5D-O5D
3	B	402	A1JBP	O1-C1-C2-C6
2	B	401	NDP	C2B-C1B-N9A-C8A
2	A	401	NDP	O4D-C1D-N1N-C6N
3	A	402	A1JBP	O2-C1-C2-C3
2	A	401	NDP	C5D-O5D-PN-O3
2	C	401	NDP	C2B-O2B-P2B-O2X
2	A	401	NDP	PN-O3-PA-O2A
3	B	402	A1JBP	O2-C1-C2-C6
2	B	401	NDP	O4D-C1D-N1N-C2N
2	C	401	NDP	C2D-C1D-N1N-C2N
2	A	401	NDP	C5D-O5D-PN-O2N
3	A	402	A1JBP	O1-C1-C2-C6
2	C	401	NDP	O4D-C1D-N1N-C2N

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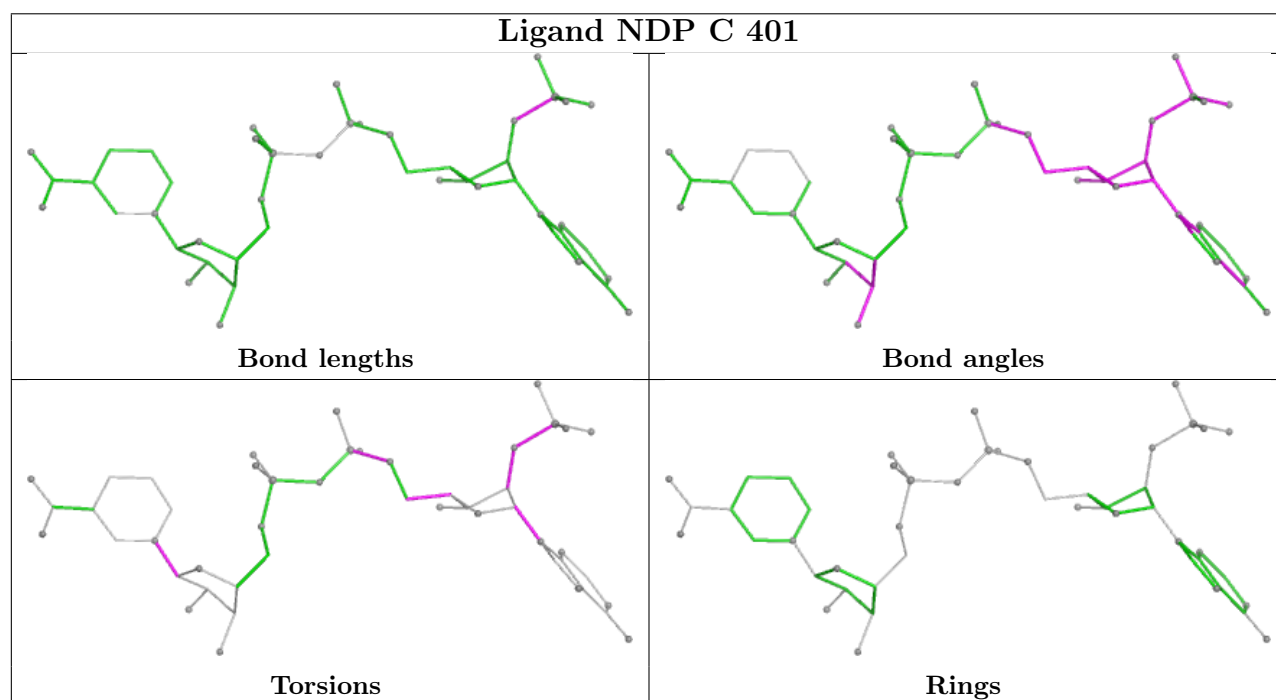
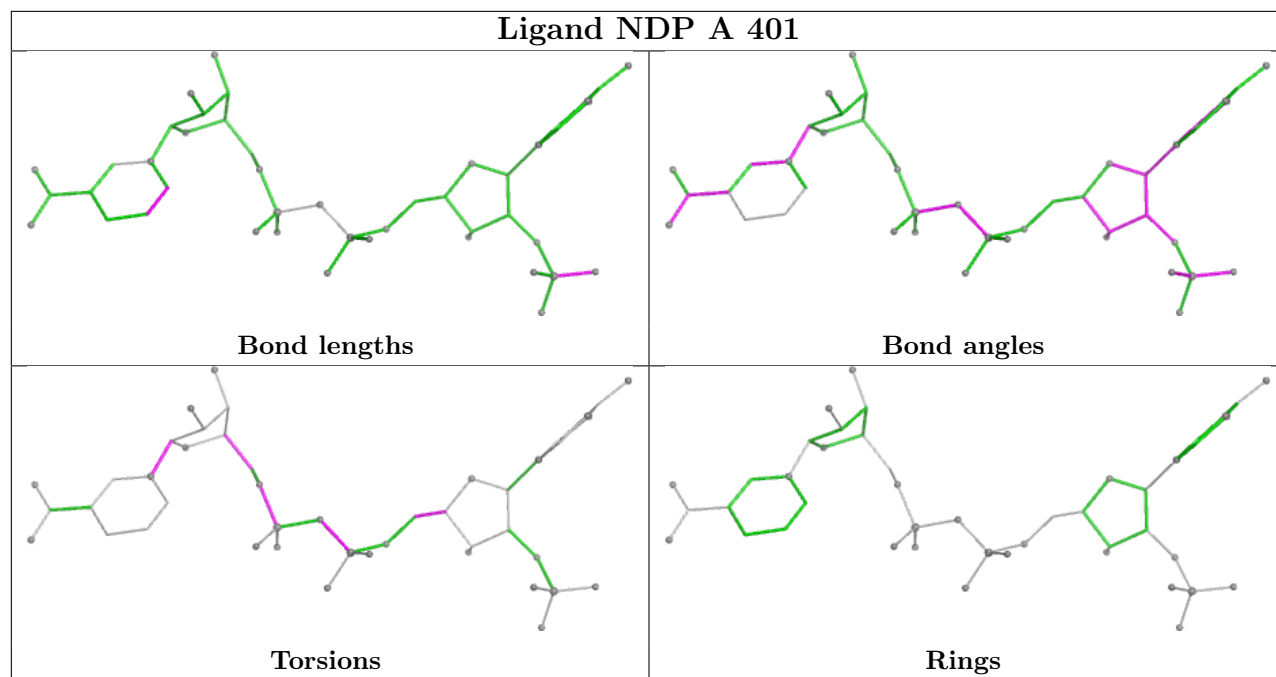
Mol	Chain	Res	Type	Atoms
2	A	401	NDP	O4D-C1D-N1N-C2N
2	B	401	NDP	O4D-C1D-N1N-C6N
2	B	401	NDP	PN-O3-PA-O2A
2	B	401	NDP	C2D-C1D-N1N-C2N
2	B	401	NDP	C3D-C4D-C5D-O5D
2	C	401	NDP	C1B-C2B-O2B-P2B
2	B	401	NDP	C2D-C1D-N1N-C6N
2	C	401	NDP	C2B-O2B-P2B-O1X
2	B	401	NDP	O4B-C1B-N9A-C8A
2	A	401	NDP	O4D-C4D-C5D-O5D
2	C	401	NDP	C2D-C1D-N1N-C6N
2	C	401	NDP	O4D-C1D-N1N-C6N
2	B	401	NDP	PN-O3-PA-O1A
2	B	401	NDP	C5B-O5B-PA-O1A
2	B	401	NDP	C5D-O5D-PN-O1N
2	C	401	NDP	C5B-O5B-PA-O2A
2	A	401	NDP	O4B-C4B-C5B-O5B
2	B	401	NDP	O4B-C4B-C5B-O5B
3	A	402	A1JBP	O2-C1-C2-C6

There are no ring outliers.

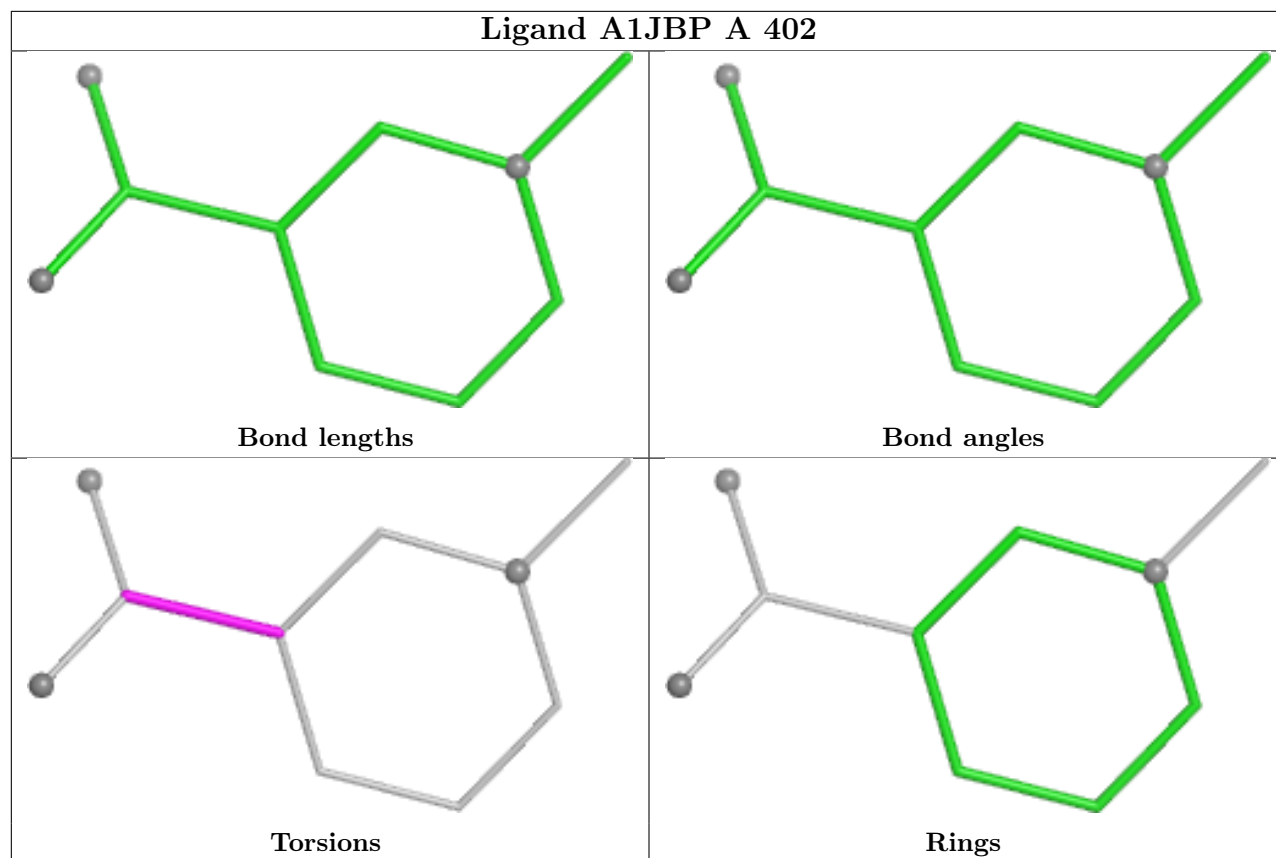
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NDP	1	0
2	C	401	NDP	2	0

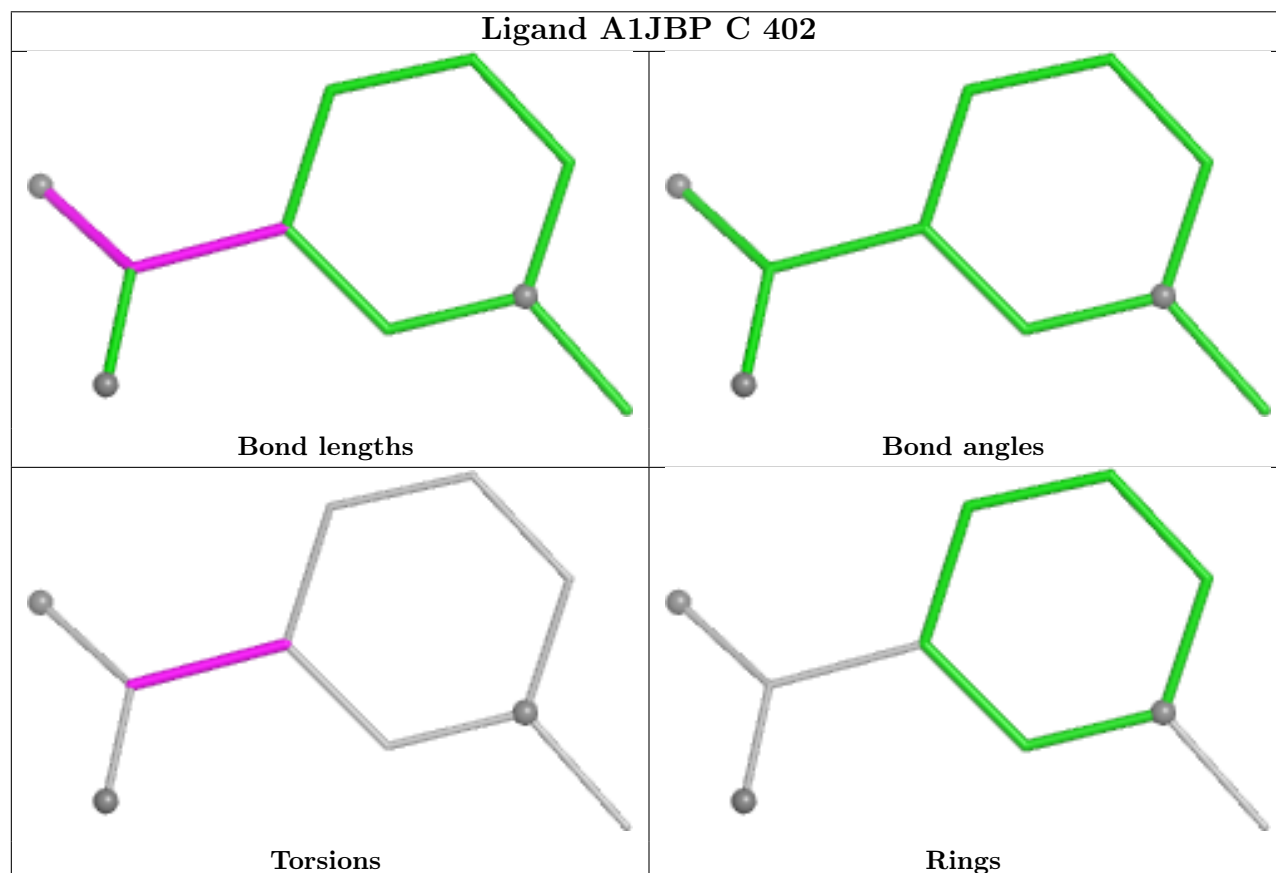
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

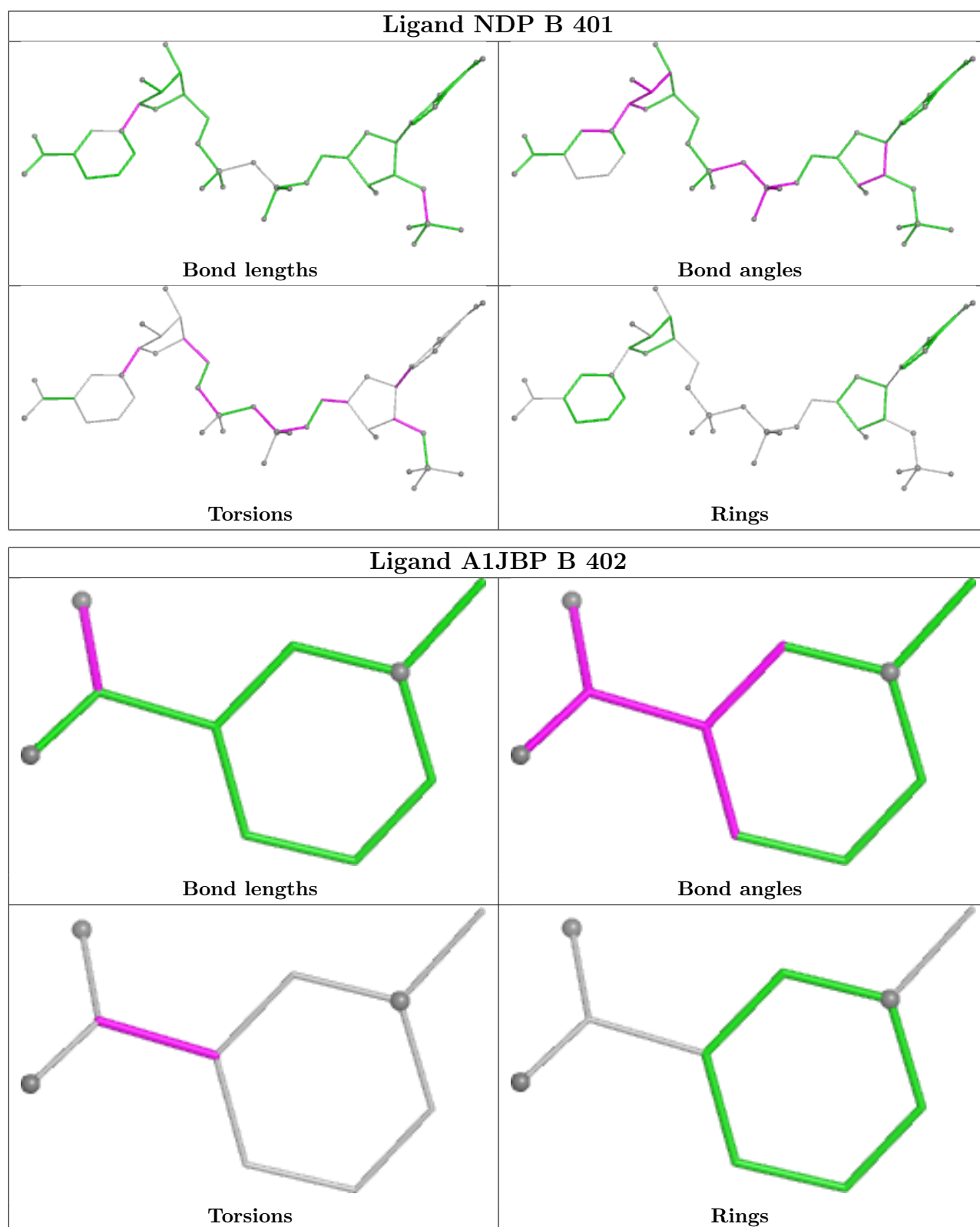


Ligand A1JBP A 402



Ligand A1JBP C 402





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	306/310 (98%)	-0.48	0 100 100	28, 49, 75, 93	0
1	B	306/310 (98%)	-0.28	1 (0%) 90 88	35, 54, 79, 104	0
1	C	306/310 (98%)	0.18	5 (1%) 70 66	40, 72, 108, 150	0
All	All	918/930 (98%)	-0.20	6 (0%) 84 82	28, 58, 100, 150	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36	LEU	3.5
1	C	37	ILE	2.7
1	C	63	PHE	2.4
1	C	54	PHE	2.4
1	C	34	PHE	2.3
1	B	252	HIS	2.3

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](#)

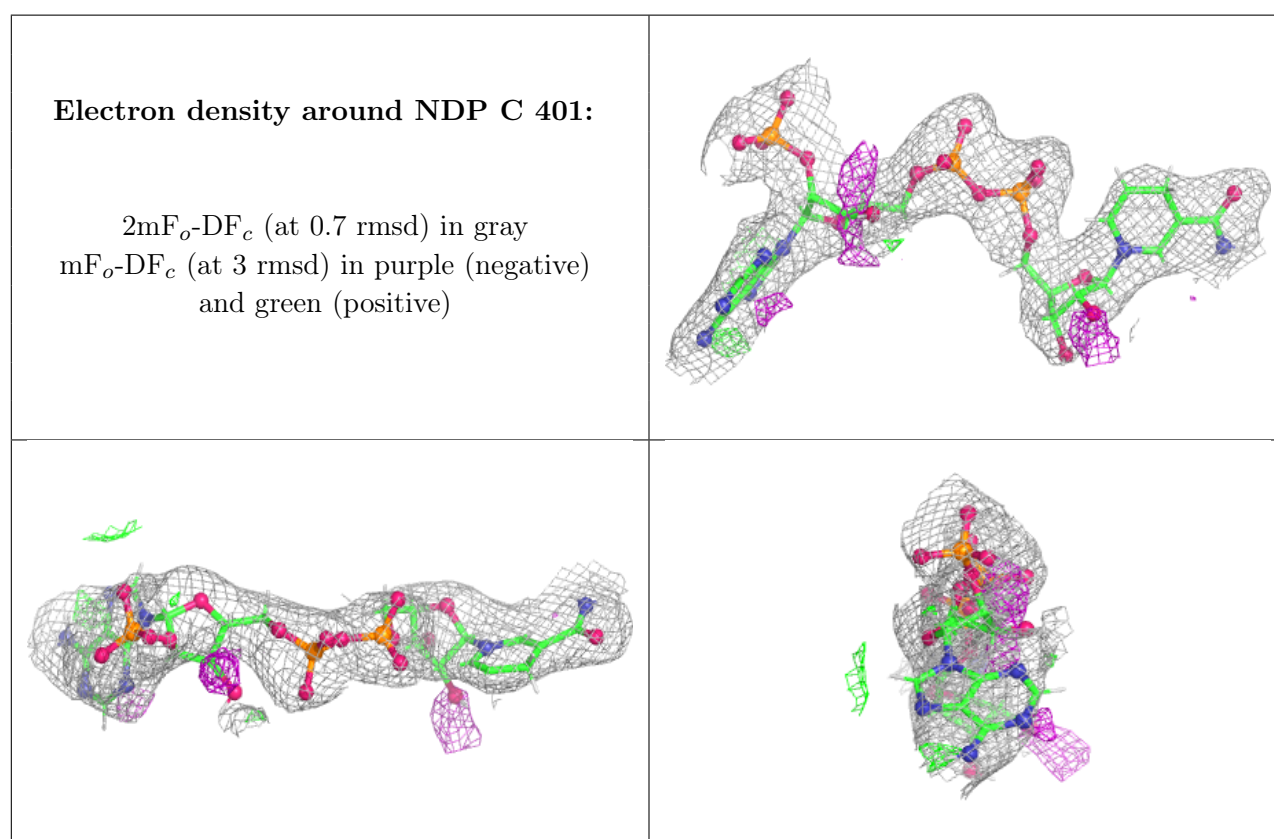
There are no oligosaccharides in this entry.

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.

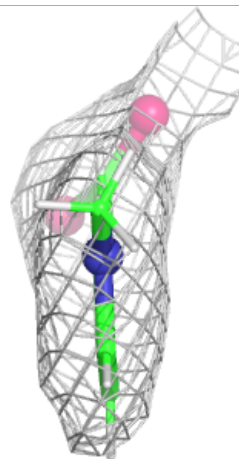
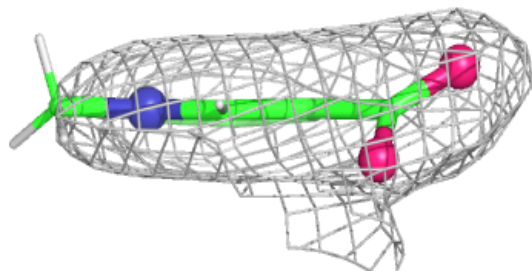
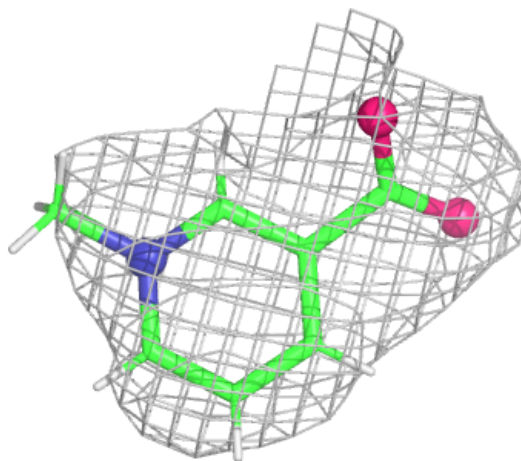
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NDP	C	401	48/48	0.92	0.10	30,64,87,92	3
3	A1JBP	B	402	10/10	0.94	0.09	30,50,58,62	3
3	A1JBP	C	402	10/10	0.96	0.13	30,51,53,54	3
2	NDP	B	401	48/48	0.97	0.06	30,36,43,48	3
2	NDP	A	401	48/48	0.97	0.06	28,33,50,52	3
3	A1JBP	A	402	10/10	0.98	0.07	30,39,43,48	3

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



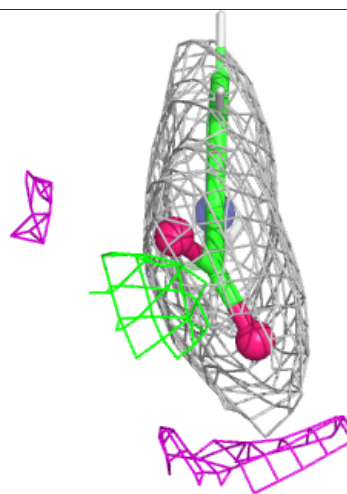
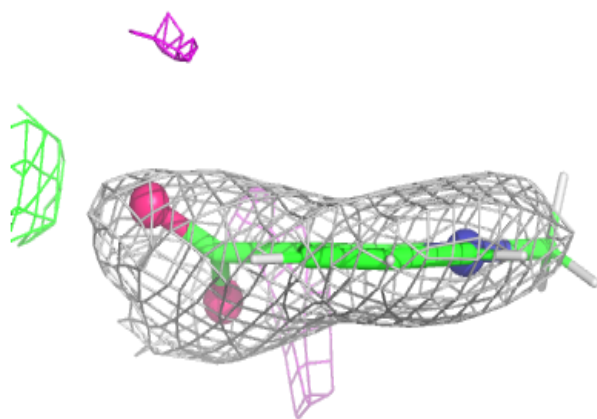
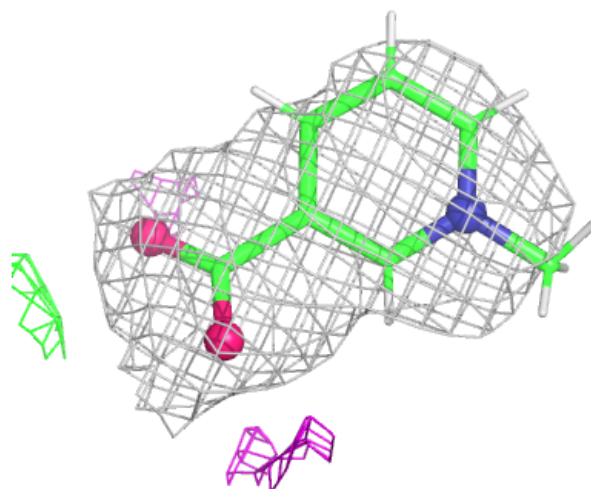
Electron density around A1JBP B 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



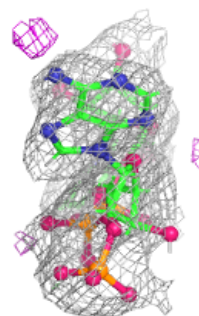
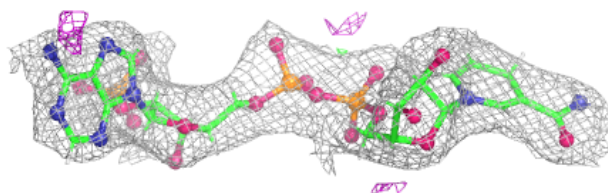
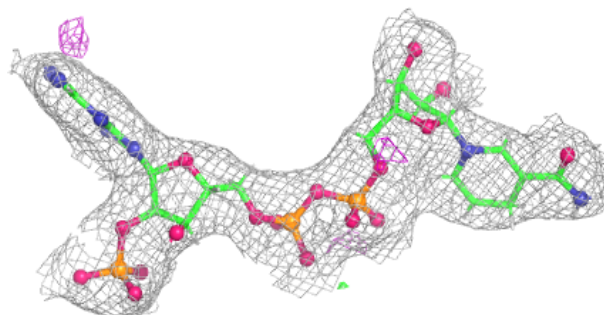
Electron density around A1JBP C 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

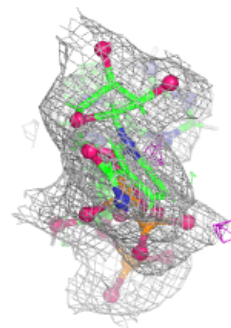
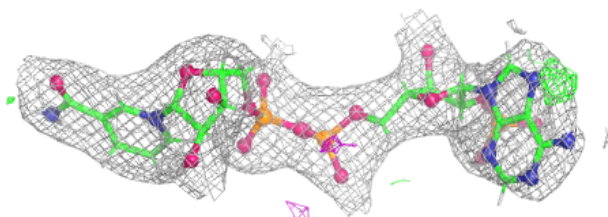
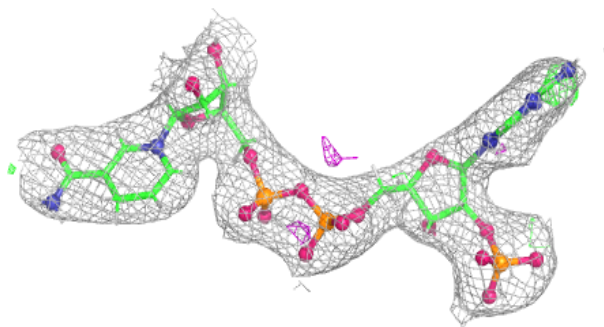


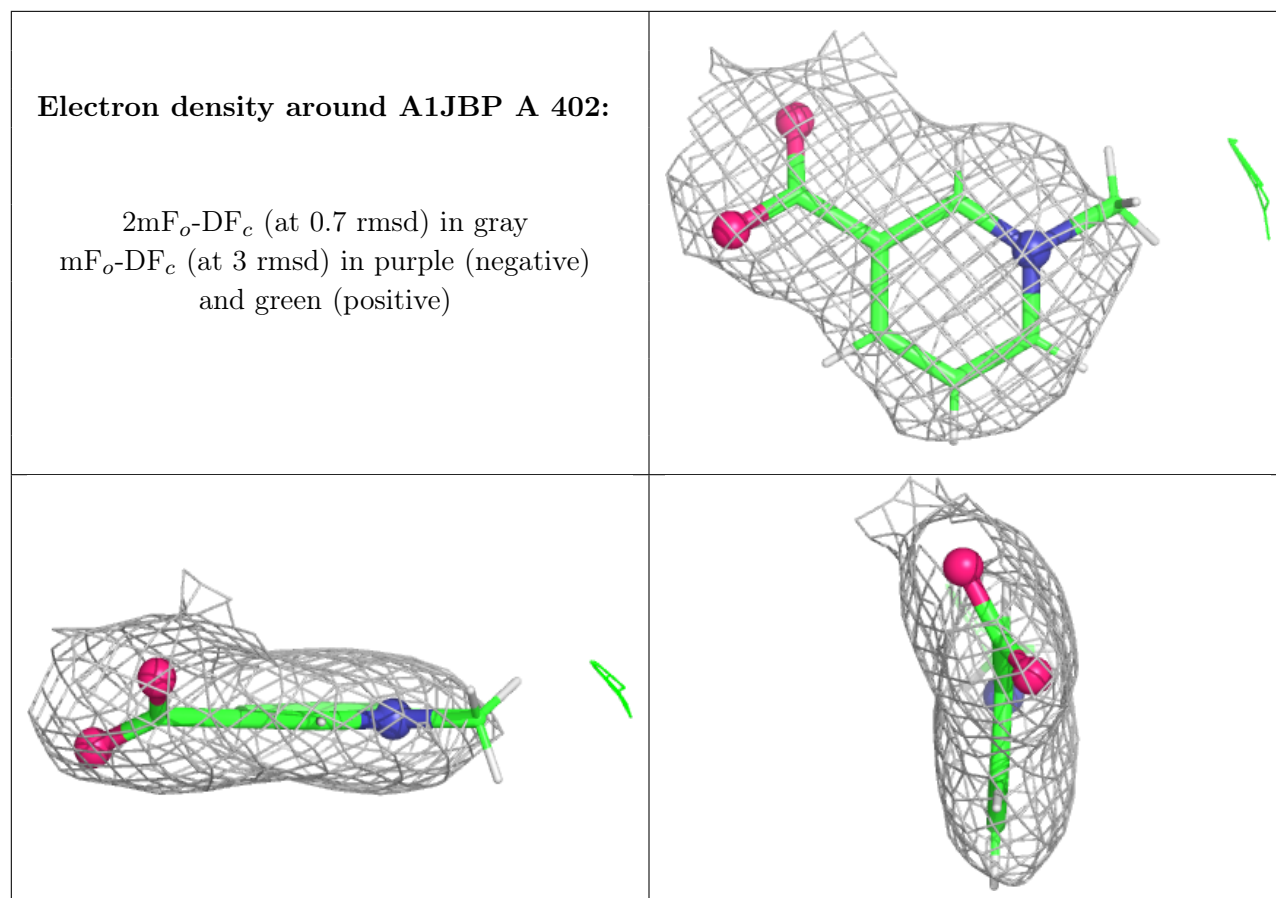
Electron density around NDP B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NDP A 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.