



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 04:41 PM EDT

PDB ID : 5V7G
Title : Crystal structure of NADPH-dependent glyoxylate/hydroxypyruvate reductase SMc04462 (SmGhrB) from *Sinorhizobium meliloti* in complex with NADPH and oxalate
Authors : Shabalin, I.G.; Mason, D.V.; Handing, K.B.; Kutner, J.; Matelska, D.; Cooper, D.R.; Bonanno, J.; Almo, S.C.; Minor, W.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : 2017-03-20
Resolution : 1.75 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

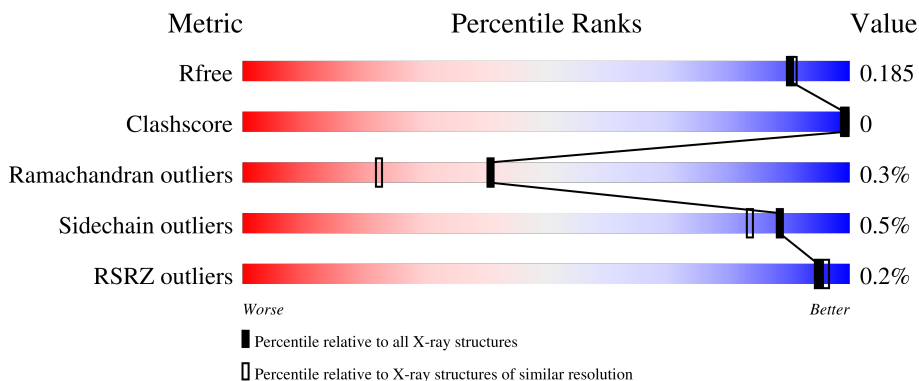
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

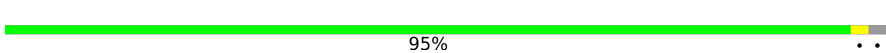
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	323	96%
1	B	323	97%
1	C	323	96%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
1	D	323	 95%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OXL	A	401	-	X	-	-
2	OXL	C	401	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11494 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.

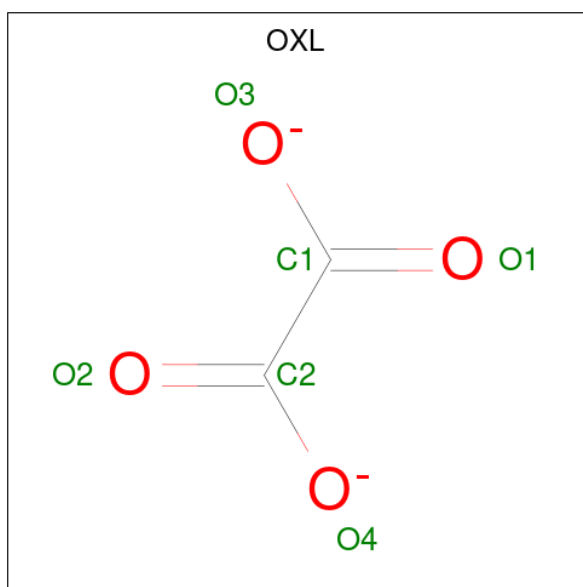
- Molecule 1 is a protein called NADPH-dependent glyoxylate/hydroxypyruvate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2347	1496	414	432	5	0	1	0
1	B	317	2361	1502	418	436	5	0	0	0
1	C	317	2365	1505	422	433	5	0	1	0
1	D	317	2375	1511	421	438	5	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

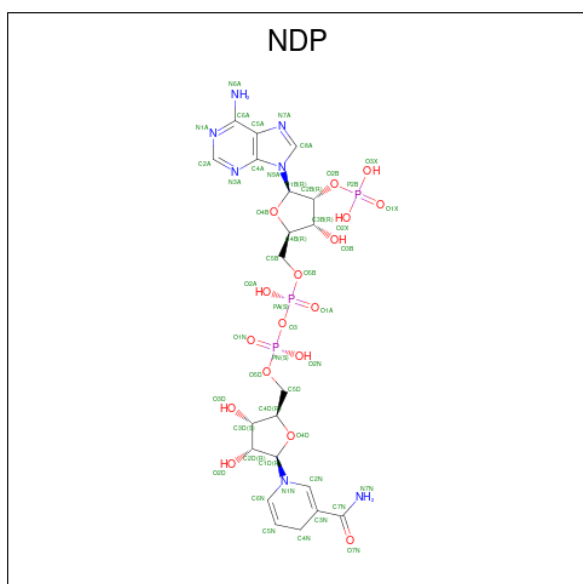
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q92LZ4
B	0	SER	-	expression tag	UNP Q92LZ4
C	0	SER	-	expression tag	UNP Q92LZ4
D	0	SER	-	expression tag	UNP Q92LZ4

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



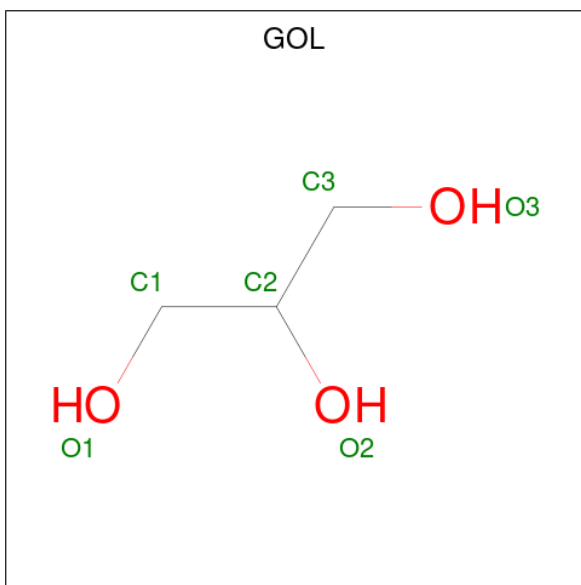
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 2 4	0	0
2	B	1	Total C O 6 2 4	0	0
2	C	1	Total C O 6 2 4	0	0
2	D	1	Total C O 6 2 4	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			6	3 3		
4	B	1	Total	C O	0	0
			6	3 3		
4	D	1	Total	C O	0	0
			6	3 3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl	0	0
			1 1		
5	B	1	Total Cl	0	0
			1 1		
5	C	1	Total Cl	0	0
			1 1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0
6	D	1	Total Na 1 1	0	0

- Molecule 7 is water.

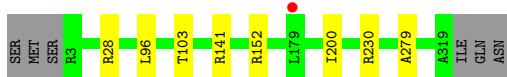
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	451	Total O 451 451	0	0
7	B	408	Total O 408 408	0	0
7	C	488	Total O 489 489	0	1
7	D	455	Total O 456 456	0	1

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.

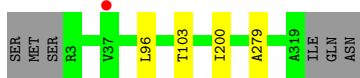
- Molecule 1: NADPH-dependent glyoxylate/hydroxypyruvate reductase

Chain A:  96%



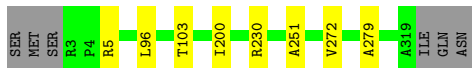
- Molecule 1: NADPH-dependent glyoxylate/hydroxypyruvate reductase

Chain B:  97%



- Molecule 1: NADPH-dependent glyoxylate/hydroxypyruvate reductase

Chain C:  96%



- Molecule 1: NADPH-dependent glyoxylate/hydroxypyruvate reductase

Chain D:  95%



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	178.21Å 178.21Å 133.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.07 – 1.75 37.07 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (37.07-1.75) 98.8 (37.07-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.150 , 0.180 0.157 , 0.185	Depositor DCC
R_{free} test set	7896 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.276 for h,-h-k,-l	Xtrriage
Reported twinning fraction	0.301 for H, K, L 0.699 for K, H, -L	Depositor
Outliers	0 of 157631 reflections	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11494	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 88.52 % 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 4.7585e-08. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, OXL, GOL, 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	0.46	0/2394	0.72	4/3274 (0.1%)
1	B	0.46	0/2404	0.71	0/3285
1	C	0.53	0/2412	0.74	2/3295 (0.1%)
1	D	0.54	0/2425	0.75	3/3313 (0.1%)
All	All	0.50	0/9635	0.73	9/13167 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	LEU	CB-CG-CD1	6.01	121.22	111.00
1	D	152	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	152	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	141	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	141	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	28	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	230	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	5	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	230	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	2347	0	2399	1	0
1	B	2361	0	2425	1	0
1	C	2365	0	2434	2	0
1	D	2375	0	2445	2	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	48	0	26	0	0
3	B	48	0	26	0	0
3	C	48	0	26	0	0
3	D	48	0	26	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	D	6	0	8	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	451	0	0	0	0
7	B	408	0	0	0	0
7	C	489	0	0	0	0
7	D	456	0	0	0	0
All	All	11494	0	9831	6	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 0.

All (6) 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:103:THR:HG21	1:A:279:ALA:HA	1.99	0.45
1:B:103:THR:HG21	1:B:279:ALA:HA	1.99	0.45
1:C:103:THR:HG21	1:C:279:ALA:HA	1.99	0.44
1:D:103:THR:HG21	1:D:279:ALA:HA	2.01	0.42
1:D:251:ALA:O	1:D:272:VAL:HA	2.21	0.41
1:C:251:ALA:O	1:C:272:VAL:HA	2.20	0.41

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	316/323 (98%)	308 (98%)	7 (2%)	1 (0%)	41 22
1	B	315/323 (98%)	307 (98%)	7 (2%)	1 (0%)	41 22
1	C	316/323 (98%)	307 (97%)	8 (2%)	1 (0%)	41 22
1	D	317/323 (98%)	309 (98%)	7 (2%)	1 (0%)	41 22
All	All	1264/1292 (98%)	1231 (97%)	29 (2%)	4 (0%)	41 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	ILE
1	A	200	ILE
1	D	200	ILE
1	C	200	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	245/258 (95%)	244 (100%)	1 (0%)	91 87
1	B	249/258 (96%)	248 (100%)	1 (0%)	91 87
1	C	249/258 (96%)	248 (100%)	1 (0%)	91 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	252/258 (98%)	250 (99%)	2 (1%)	81	72
All	All	995/1032 (96%)	990 (100%)	5 (0%)	88	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LEU
1	B	96	LEU
1	C	96	LEU
1	D	36	LEU
1	D	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 for Mogul analysis.

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	OXL	B	401	-	5,5,5	1.71	1 (20%)	6,6,6	1.25	0
2	OXL	C	401	-	5,5,5	1.55	1 (20%)	6,6,6	1.92	2 (33%)
3	NDP	B	402	-	45,52,52	1.23	1 (2%)	53,80,80	1.22	4 (7%)
3	NDP	C	402	-	45,52,52	1.29	3 (6%)	53,80,80	1.20	4 (7%)
3	NDP	A	402	-	45,52,52	1.24	1 (2%)	53,80,80	1.17	2 (3%)
4	GOL	B	403	-	5,5,5	0.28	0	5,5,5	0.26	0
4	GOL	D	403	-	5,5,5	0.29	0	5,5,5	0.37	0
4	GOL	A	403	-	5,5,5	0.30	0	5,5,5	0.20	0
3	NDP	D	402	-	45,52,52	1.27	3 (6%)	53,80,80	1.13	2 (3%)
2	OXL	D	401	-	5,5,5	1.68	1 (20%)	6,6,6	1.13	0
2	OXL	A	401	-	5,5,5	1.77	1 (20%)	6,6,6	1.50	2 (33%)

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	OXL	B	401	-	-	4/4/4/4	-
2	OXL	C	401	-	-	4/4/4/4	-
3	NDP	B	402	-	-	2/30/77/77	0/5/5/5
3	NDP	C	402	-	-	2/30/77/77	0/5/5/5
3	NDP	A	402	-	-	2/30/77/77	0/5/5/5
4	GOL	B	403	-	-	0/4/4/4	-
4	GOL	D	403	-	-	3/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
3	NDP	D	402	-	-	5/30/77/77	0/5/5/5
2	OXL	D	401	-	-	4/4/4/4	-
2	OXL	A	401	-	-	4/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NDP	C8A-N7A	6.92	1.47	1.34
3	D	402	NDP	C8A-N7A	6.57	1.46	1.34
3	C	402	NDP	C8A-N7A	6.53	1.46	1.34
3	B	402	NDP	C8A-N7A	6.50	1.46	1.34
2	A	401	OXL	C2-C1	-2.79	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NDP	O4B-C1B	2.57	1.44	1.41
2	B	401	OXL	C2-C1	-2.52	1.47	1.54
3	D	402	NDP	P2B-O2B	2.33	1.63	1.59
3	C	402	NDP	C2A-N3A	2.26	1.35	1.32
2	D	401	OXL	C2-C1	-2.22	1.48	1.54
3	D	402	NDP	C2A-N3A	2.04	1.35	1.32
2	C	401	OXL	C2-C1	-2.04	1.48	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NDP	N3A-C2A-N1A	-5.21	120.54	128.68
3	B	402	NDP	N3A-C2A-N1A	-4.90	121.03	128.68
3	C	402	NDP	N3A-C2A-N1A	-4.74	121.28	128.68
3	D	402	NDP	N3A-C2A-N1A	-4.71	121.32	128.68
2	C	401	OXL	O4-C2-C1	3.28	122.90	113.16
3	C	402	NDP	O2B-P2B-O1X	-2.61	99.33	109.39
2	A	401	OXL	O4-C2-C1	2.48	120.53	113.16
2	C	401	OXL	O3-C1-C2	2.39	120.25	113.16
3	B	402	NDP	C3N-C2N-N1N	-2.34	119.76	123.10
3	A	402	NDP	C3D-C2D-C1D	2.31	105.81	101.43
3	C	402	NDP	C3N-C2N-N1N	-2.30	119.81	123.10
3	C	402	NDP	C3D-C2D-C1D	2.21	105.62	101.43
2	A	401	OXL	O3-C1-C2	2.17	119.61	113.16
3	B	402	NDP	O7N-C7N-C3N	-2.17	116.81	120.90
3	D	402	NDP	PN-O3-PA	-2.10	125.64	132.83
3	B	402	NDP	O2N-PN-O1N	2.04	122.32	112.24

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	OXL	O1-C1-C2-O2
2	A	401	OXL	O3-C1-C2-O2
2	A	401	OXL	O3-C1-C2-O4
2	B	401	OXL	O1-C1-C2-O2
2	B	401	OXL	O1-C1-C2-O4
2	B	401	OXL	O3-C1-C2-O2
2	B	401	OXL	O3-C1-C2-O4
2	D	401	OXL	O1-C1-C2-O2
2	D	401	OXL	O1-C1-C2-O4
2	D	401	OXL	O3-C1-C2-O2

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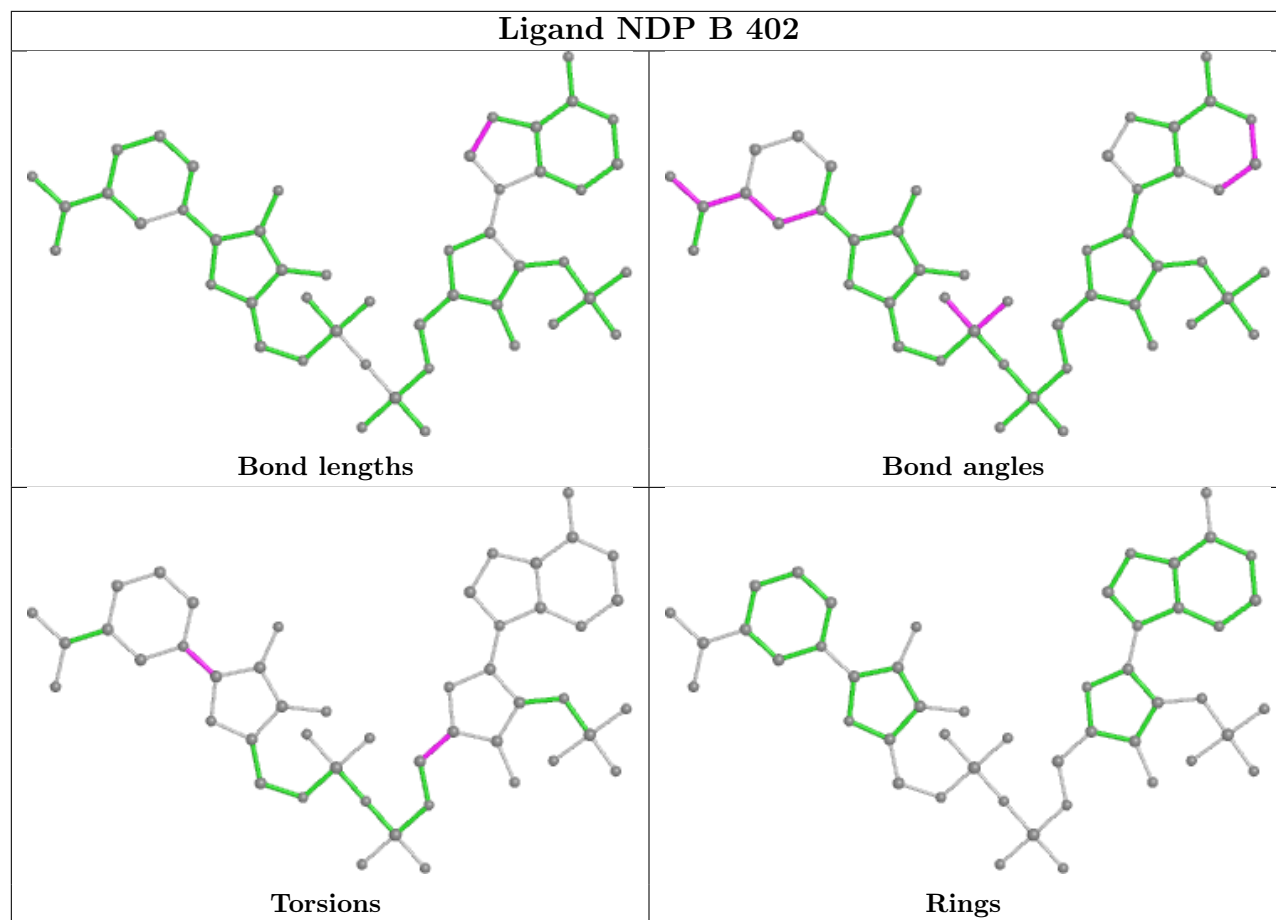
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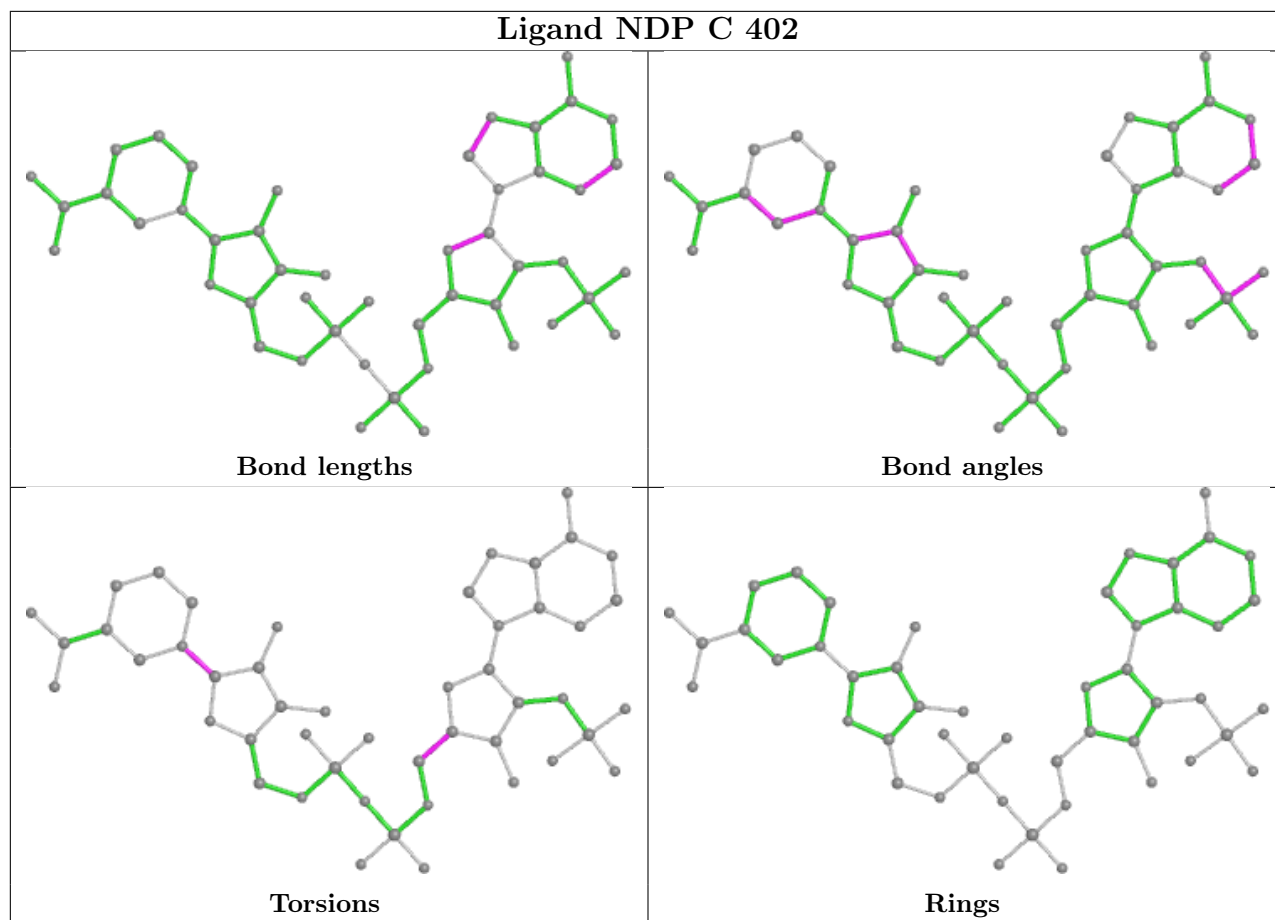
Mol	Chain	Res	Type	Atoms
2	D	401	OXL	O3-C1-C2-O4
3	D	402	NDP	C2B-O2B-P2B-O2X
3	D	402	NDP	C2N-C3N-C7N-N7N
4	A	403	GOL	C1-C2-C3-O3
4	D	403	GOL	O2-C2-C3-O3
2	A	401	OXL	O1-C1-C2-O4
2	C	401	OXL	O1-C1-C2-O2
2	C	401	OXL	O3-C1-C2-O4
4	A	403	GOL	O2-C2-C3-O3
2	C	401	OXL	O1-C1-C2-O4
4	D	403	GOL	O1-C1-C2-C3
4	D	403	GOL	C1-C2-C3-O3
2	C	401	OXL	O3-C1-C2-O2
3	C	402	NDP	O4D-C1D-N1N-C2N
3	A	402	NDP	O4D-C1D-N1N-C2N
3	D	402	NDP	C2B-O2B-P2B-O1X
3	B	402	NDP	O4D-C1D-N1N-C2N
3	D	402	NDP	O4D-C1D-N1N-C2N
3	D	402	NDP	O4B-C4B-C5B-O5B
3	A	402	NDP	O4B-C4B-C5B-O5B
3	B	402	NDP	O4B-C4B-C5B-O5B
3	C	402	NDP	O4B-C4B-C5B-O5B

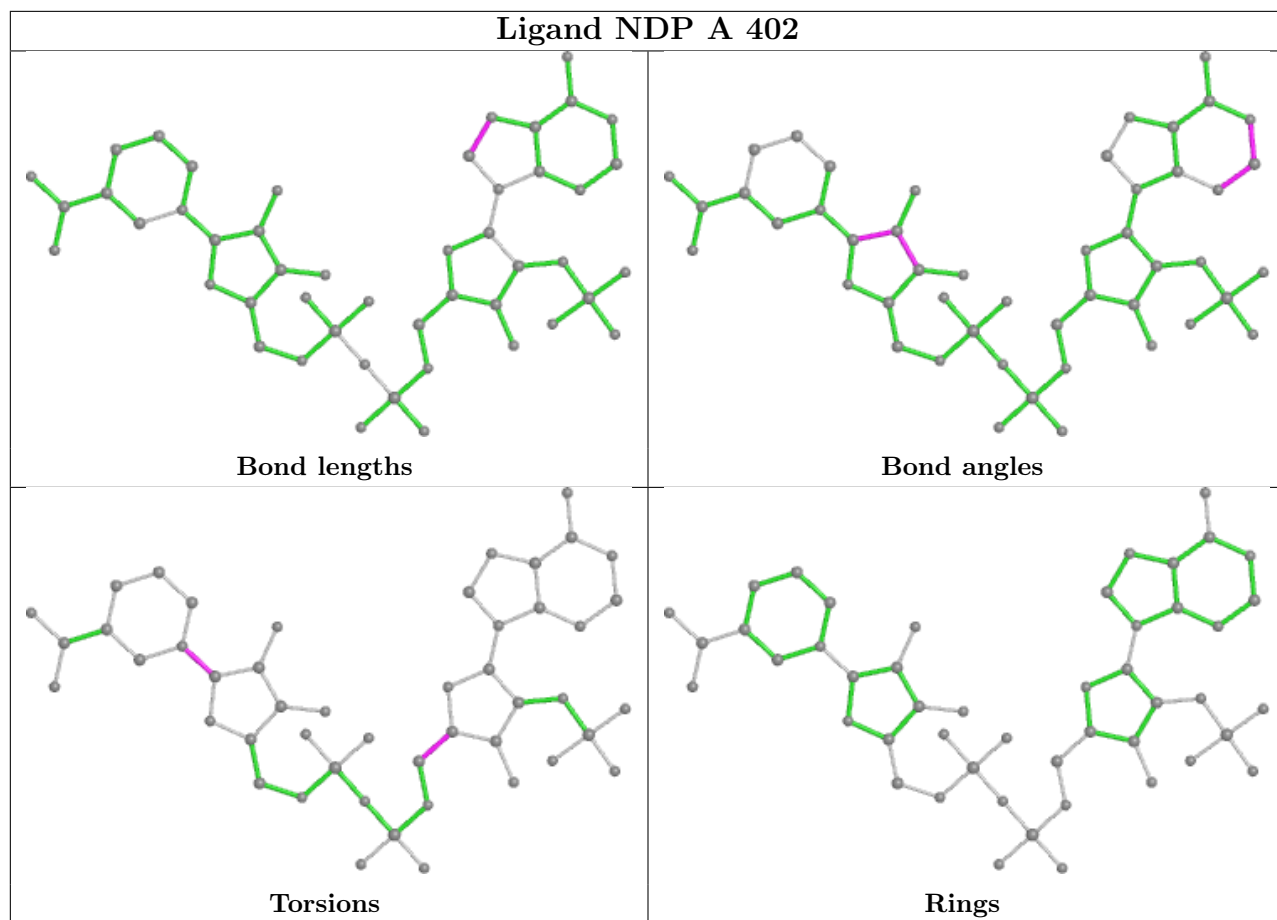
There are no ring outliers.

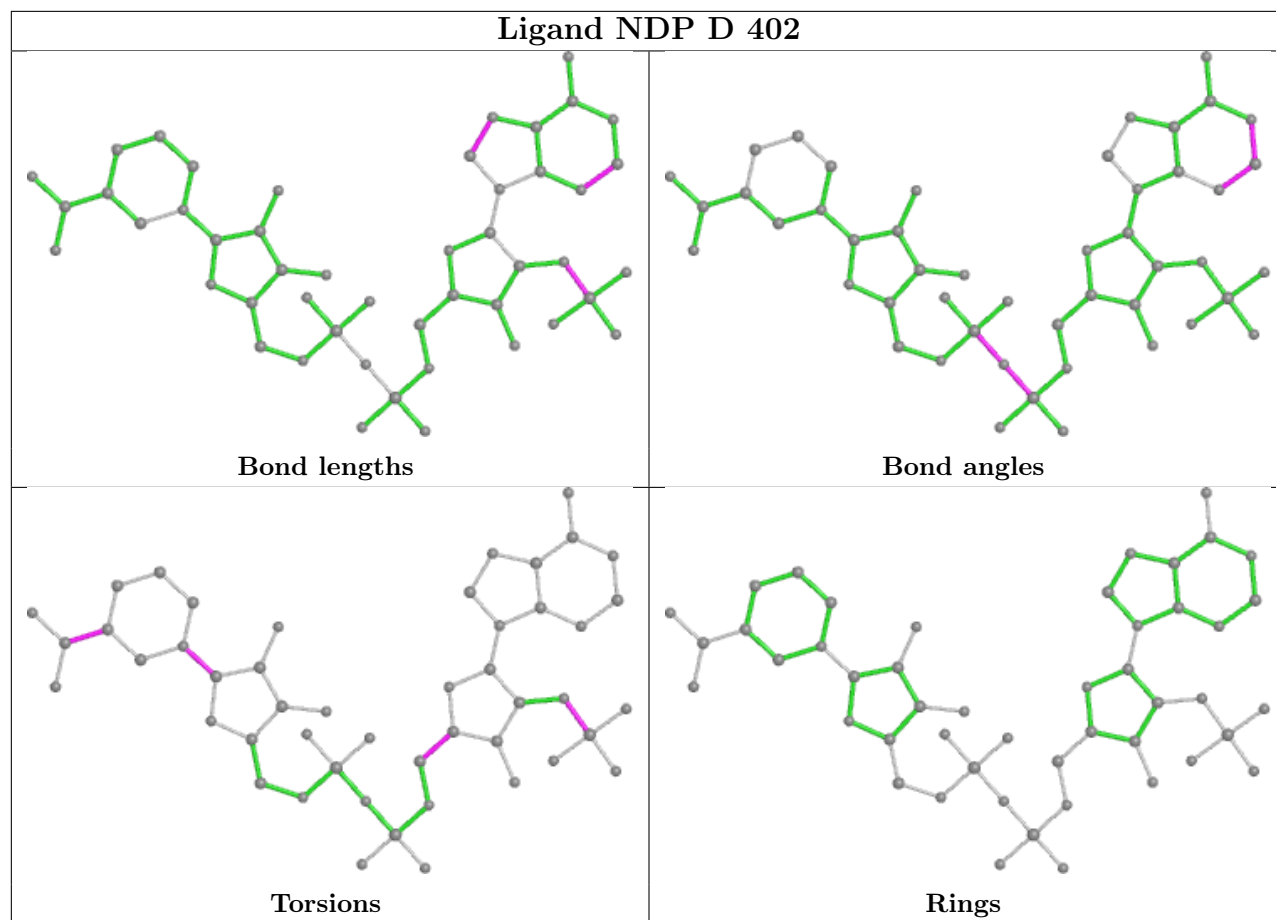
No monomer is involved in short contacts.

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	317/323 (98%)	-0.47	1 (0%) 94 95	20, 31, 47, 74	0
1	B	317/323 (98%)	-0.37	1 (0%) 94 95	22, 33, 49, 85	0
1	C	317/323 (98%)	-0.56	0 100 100	14, 23, 41, 62	0
1	D	317/323 (98%)	-0.45	0 100 100	14, 25, 43, 69	0
All	All	1268/1292 (98%)	-0.46	2 (0%) 95 96	14, 28, 46, 85	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	VAL	2.5
1	A	179	LEU	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](#)

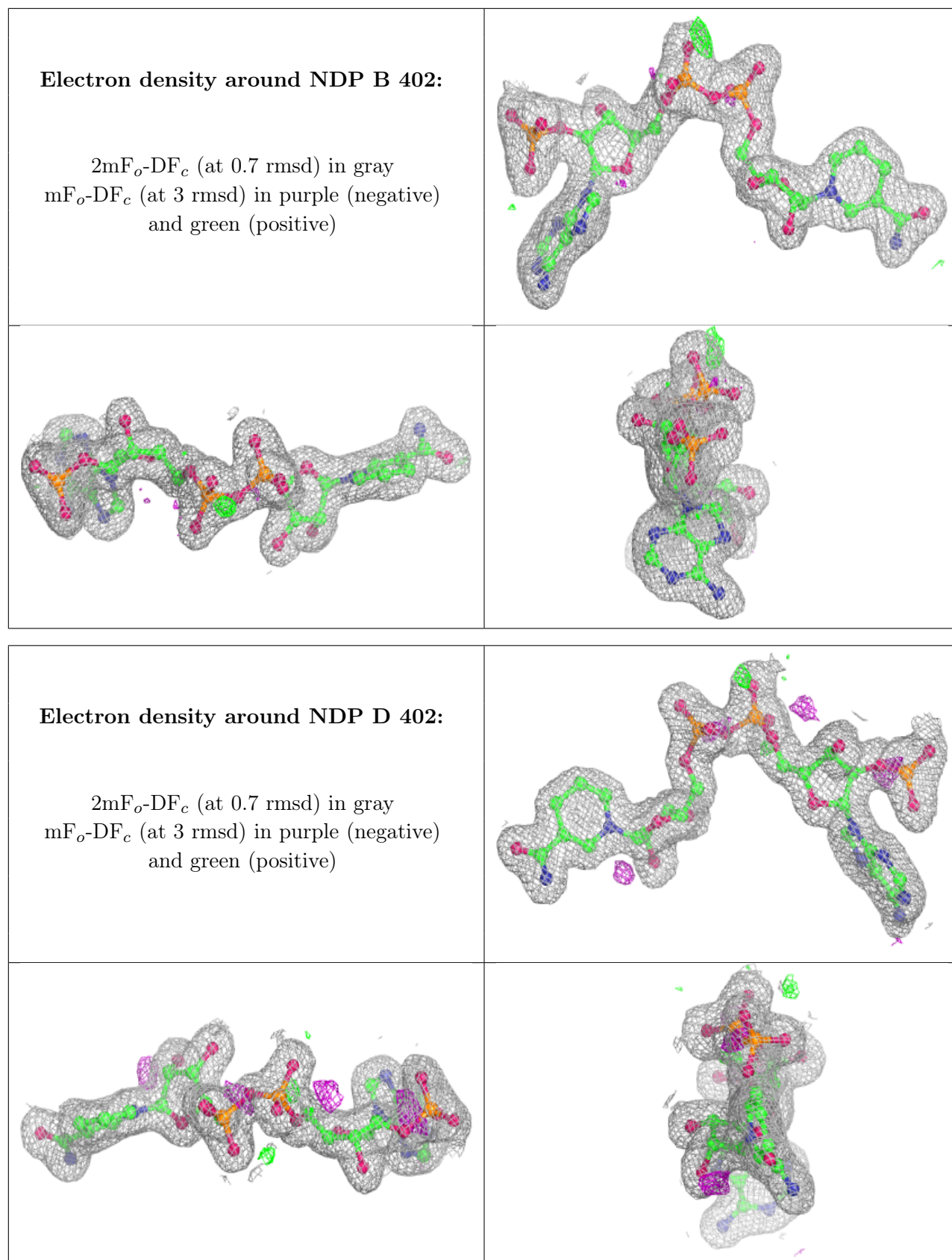
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

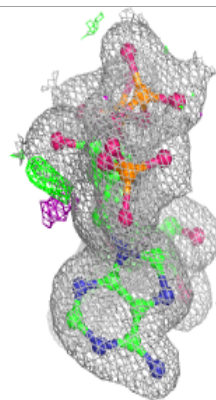
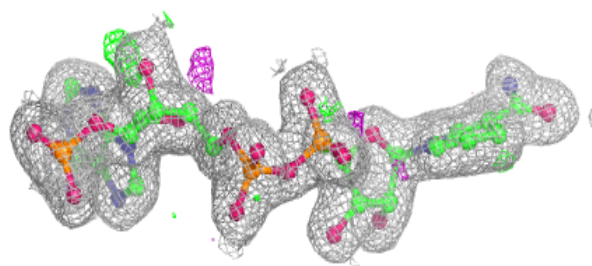
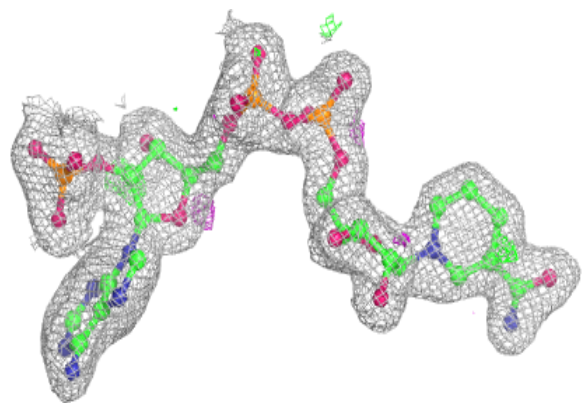
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	403	6/6	0.92	0.11	22,38,45,57	6
6	NA	D	405	1/1	0.93	0.07	29,29,29,29	0
2	OXL	A	401	6/6	0.95	0.07	23,28,37,52	6
6	NA	B	405	1/1	0.95	0.04	34,34,34,34	0
4	GOL	A	403	6/6	0.95	0.09	22,30,45,55	6
4	GOL	D	403	6/6	0.96	0.12	21,27,48,60	6
6	NA	A	405	1/1	0.96	0.06	38,38,38,38	0
2	OXL	B	401	6/6	0.96	0.08	18,23,36,48	6
2	OXL	C	401	6/6	0.96	0.08	16,18,26,26	6
6	NA	C	404	1/1	0.97	0.06	26,26,26,26	0
3	NDP	B	402	48/48	0.97	0.07	23,29,37,42	0
3	NDP	D	402	48/48	0.98	0.07	13,21,27,28	0
3	NDP	A	402	48/48	0.98	0.07	19,28,37,47	0
2	OXL	D	401	6/6	0.98	0.07	20,25,30,36	0
3	NDP	C	402	48/48	0.98	0.07	13,19,26,28	0
5	CL	A	404	1/1	0.99	0.04	36,36,36,36	0
5	CL	B	404	1/1	0.99	0.10	38,38,38,38	0
5	CL	C	403	1/1	0.99	0.04	27,27,27,27	0
5	CL	D	404	1/1	0.99	0.03	31,31,31,31	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.

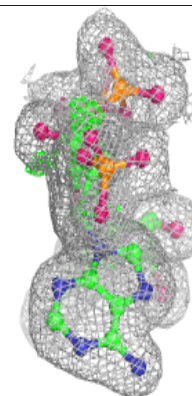
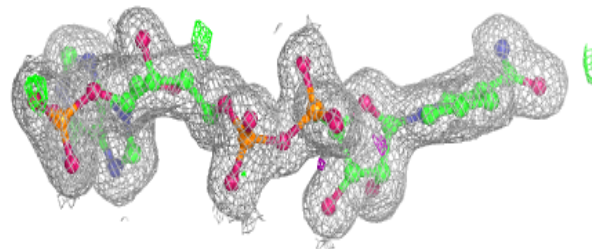
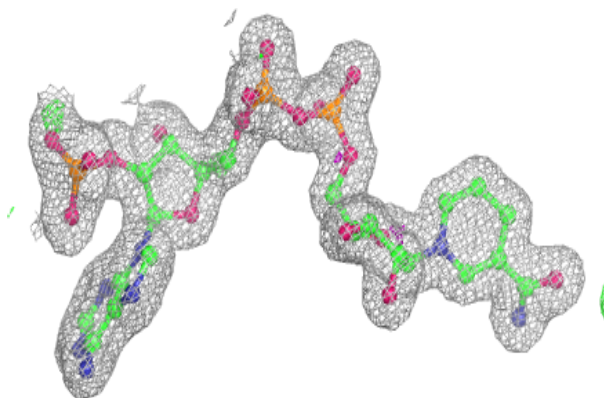


Electron density around NDP A 402:

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

**Electron density around NDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.