



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:16 AM UTC

PDB ID : 3A06 / pdb_00003a06
Title : Crystal structure of DXR from *Thermooga maritima*, in complex with fosmidomycin and NADPH
Authors : Takenoya, M.; Ohtaki, A.; Noguchi, K.; Sasaki, Y.; Ohsawa, K.; Yohda, M.; Yajima, S.
Deposited on : 2009-03-02
Resolution : 2.00 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

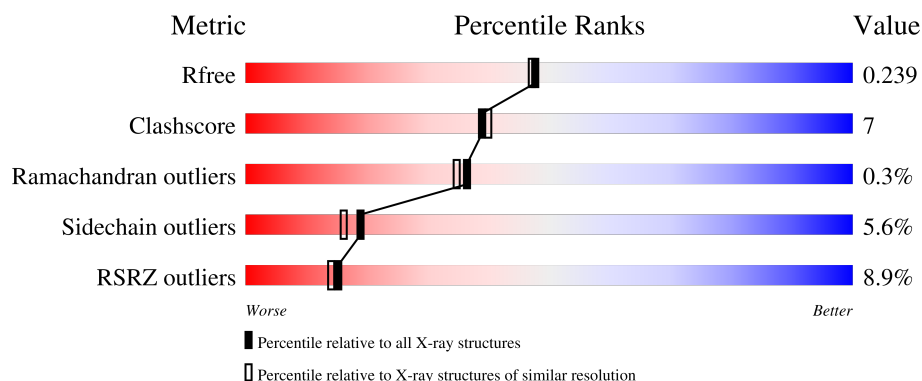
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	376	11% 83% 12% ..
1	B	376	7% 85% 12% ..

2 Entry composition [i](#)

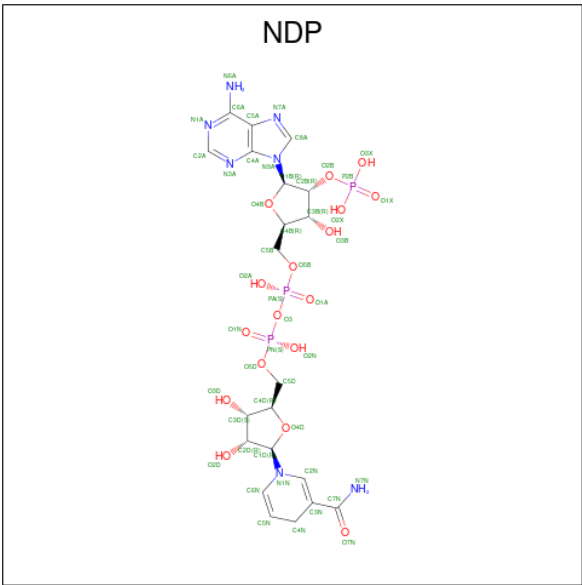
There are 5 unique types of molecules in this entry. The entry contains 6130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	3	0
			2932	1888	496	538	10			
1	B	373	Total	C	N	O	S	0	1	0
			2950	1899	499	542	10			

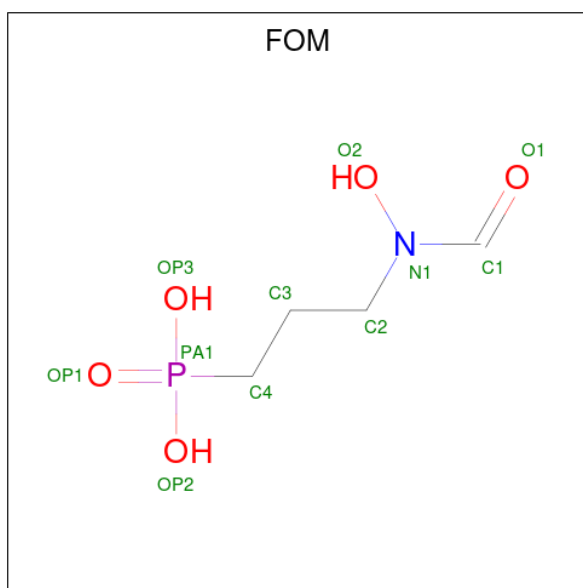
- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3-[FORMYL(HYDROXY)AMINO]PROPYLPHOSPHONIC ACID (CCD ID:

FOM) (formula: C₄H₁₀NO₅P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			5	1	3	1		
3	B	1	Total	C	O	P	0	0
			5	1	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

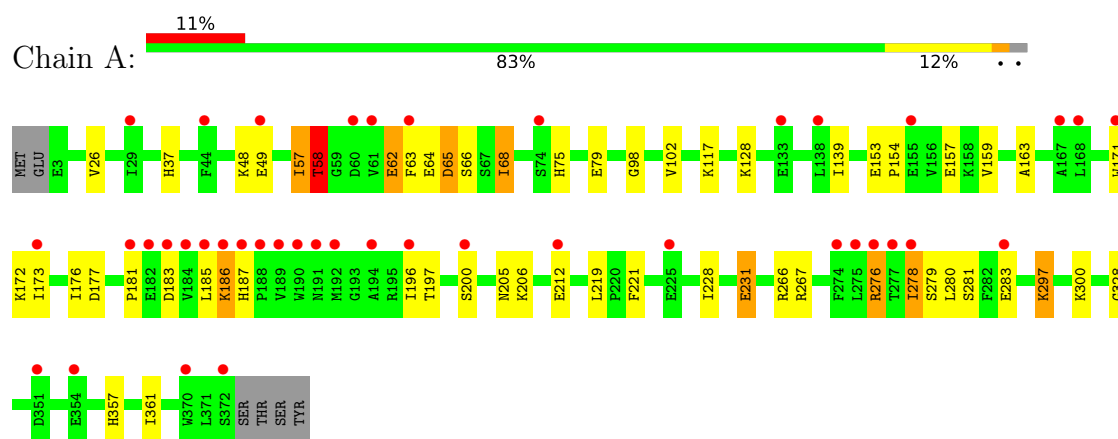
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	54	Total	O	0	0
			54	54		

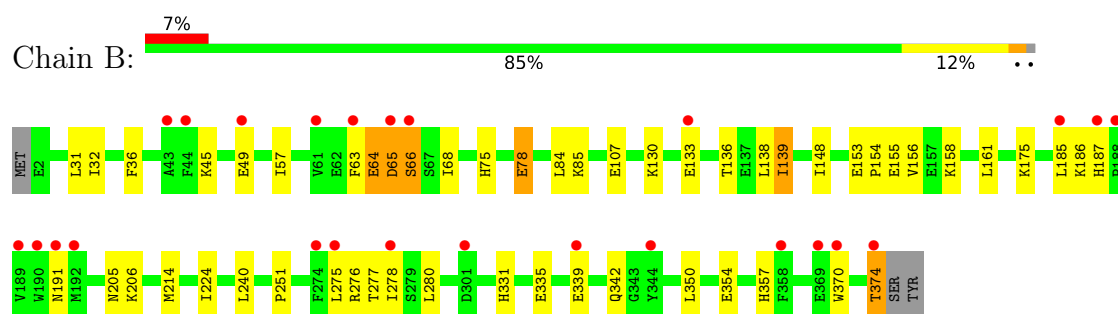
3 Residue-property plots [i](#)

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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	108.62Å 108.62Å 74.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.72 – 2.00 40.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.72-2.00) 99.5 (40.72-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.62 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.240 0.207 , 0.239	Depositor DCC
R_{free} test set	2953 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6130	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: MG, NDP, FOM

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	0.76	1/3007 (0.0%)	0.91	2/4061 (0.0%)
1	B	0.73	1/3014 (0.0%)	0.89	2/4071 (0.0%)
All	All	0.75	2/6021 (0.0%)	0.90	4/8132 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	PRO	CA-C	5.79	1.55	1.51
1	A	139	ILE	CA-CB	5.65	1.58	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	THR	N-CA-C	-5.50	107.21	114.31
1	B	65	ASP	CA-C-N	5.34	131.31	121.70
1	B	65	ASP	C-N-CA	5.34	131.31	121.70
1	A	57	ILE	CB-CA-C	-5.11	103.89	110.84

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	2932	0	3005	46	0
1	B	2950	0	3024	38	0
2	A	75	0	37	2	0
2	B	48	0	26	1	0
3	A	5	0	0	4	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	59	0	0	4	0
5	B	54	0	0	1	0
All	All	6130	0	6092	82	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 (82) 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:65:ASP:HB3	1:A:66:SER:HA	1.15	1.09
1:A:205[B]:ASN:ND2	3:A:900:FOM:OP1	1.91	1.04
1:A:65:ASP:HB3	1:A:66:SER:CA	1.89	1.03
1:A:117:LYS:HB3	1:A:212:GLU:OE1	1.64	0.96
1:A:65:ASP:CB	1:A:66:SER:HA	2.02	0.90
1:A:58:THR:HG21	2:A:3001:NDP:C2A	2.02	0.90
1:B:148:ILE:HD11	1:B:161:LEU:CD2	2.09	0.81
1:B:65:ASP:HB2	1:B:66:SER:HB2	1.68	0.74
1:B:148:ILE:HD11	1:B:161:LEU:HD23	1.69	0.74
1:A:117:LYS:CB	1:A:212:GLU:OE1	2.36	0.72
1:A:75:HIS:O	1:A:79:GLU:HG3	1.92	0.69
1:B:331:HIS:HD2	1:B:335:GLU:OE2	1.76	0.69
1:A:357:HIS:HD2	5:A:382:HOH:O	1.75	0.69
1:B:139:ILE:N	1:B:139:ILE:HD12	2.09	0.68
1:A:63:PHE:HE2	1:A:68:ILE:HD11	1.57	0.68
1:B:357:HIS:HD2	5:B:406:HOH:O	1.78	0.66
1:A:117:LYS:HE3	1:A:205[A]:ASN:OD1	1.99	0.63
3:A:900:FOM:C4	5:A:602:HOH:O	2.49	0.60
1:A:63:PHE:CE2	1:A:68:ILE:HD11	2.38	0.58
1:A:205[B]:ASN:HD21	3:A:900:FOM:PA1	2.27	0.57
1:B:370:TRP:O	1:B:374:THR:HB	2.03	0.57
1:B:138:LEU:C	1:B:139:ILE:HD12	2.31	0.56
5:A:432:HOH:O	1:B:276:ARG:HG3	2.05	0.56
1:B:65:ASP:HB2	1:B:66:SER:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:HIS:ND1	1:A:58:THR:HG22	2.23	0.53
1:A:177:ASP:HB2	5:A:384:HOH:O	2.09	0.53
1:A:37:HIS:HA	1:A:58:THR:HG22	1.91	0.53
1:B:65:ASP:CB	1:B:66:SER:HA	2.38	0.53
1:A:205[B]:ASN:CG	3:A:900:FOM:OP1	2.53	0.52
1:B:185:LEU:O	1:B:186:LYS:HD2	2.07	0.52
1:A:228:ILE:HB	1:A:283:GLU:HG3	1.92	0.52
1:B:65:ASP:HB3	1:B:66:SER:HA	1.92	0.52
1:A:276:ARG:HD3	1:A:276:ARG:N	2.25	0.51
1:A:186:LYS:HB2	1:A:197:THR:HG21	1.92	0.51
1:B:205[B]:ASN:ND2	1:B:206:LYS:H	2.10	0.50
1:A:163:ALA:HB2	1:A:206:LYS:HE3	1.94	0.50
1:B:65:ASP:CB	1:B:66:SER:CA	2.90	0.49
1:A:62:GLU:N	1:A:62:GLU:OE1	2.45	0.49
1:B:153:GLU:O	1:B:156:VAL:HG13	2.13	0.49
1:B:153:GLU:HB2	1:B:154:PRO:HD2	1.96	0.48
1:B:214:MET:HG3	1:B:224:ILE:CD1	2.44	0.47
1:A:153:GLU:HB2	1:A:154:PRO:CD	2.45	0.46
1:B:75:HIS:O	1:B:78:GLU:HG2	2.15	0.46
1:A:276:ARG:HD3	1:A:276:ARG:H	1.80	0.46
1:A:231:GLU:HG3	1:A:279:SER:O	2.16	0.46
1:A:58:THR:CG2	2:A:3001:NDP:C2A	2.86	0.46
1:B:139:ILE:N	1:B:139:ILE:CD1	2.79	0.46
1:A:177:ASP:OD2	1:A:328:GLY:HA3	2.16	0.45
1:B:57:ILE:HD11	1:B:63:PHE:CB	2.47	0.45
1:B:64:GLU:HA	1:B:65:ASP:HA	1.84	0.45
1:A:280:LEU:O	1:B:277:THR:HA	2.16	0.45
1:B:148:ILE:CD1	1:B:161:LEU:CD2	2.88	0.45
1:B:339:GLU:O	1:B:342:GLN:HG3	2.16	0.45
1:A:98:GLY:O	1:A:102:VAL:HG23	2.17	0.44
1:A:163:ALA:CB	1:A:206:LYS:HE3	2.47	0.44
1:A:297:LYS:H	1:A:297:LYS:CD	2.31	0.44
1:A:63:PHE:HE2	1:A:68:ILE:CD1	2.27	0.44
1:A:205[B]:ASN:OD1	1:A:206:LYS:N	2.51	0.44
1:B:107:GLU:OE2	1:B:130:LYS:NZ	2.35	0.43
1:B:205[B]:ASN:ND2	1:B:206:LYS:N	2.67	0.43
1:A:221:PHE:CG	1:A:300:LYS:HD3	2.54	0.42
1:A:159:VAL:HG21	1:A:219:LEU:HD11	2.01	0.42
1:A:278:ILE:HG22	1:B:280:LEU:HB2	2.01	0.42
1:A:37:HIS:ND1	1:A:58:THR:CG2	2.81	0.42
1:A:171:TRP:CZ2	1:A:183:ASP:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LYS:HD3	1:B:206:LYS:HA	1.87	0.42
1:B:78:GLU:CD	1:B:78:GLU:H	2.27	0.42
1:B:57:ILE:HD11	1:B:63:PHE:HB3	2.02	0.42
2:B:3002:NDP:H71N	2:B:3002:NDP:H2N	1.68	0.41
1:B:32:ILE:HD12	1:B:84:LEU:HD22	2.01	0.41
1:A:196:ILE:H	1:A:196:ILE:HG13	1.73	0.41
1:A:231:GLU:H	1:A:231:GLU:CD	2.28	0.41
1:A:357:HIS:O	1:A:361:ILE:HG12	2.21	0.41
1:B:36:PHE:CE1	1:B:57:ILE:HG12	2.56	0.41
1:A:267:ARG:CZ	1:B:240:LEU:HD13	2.51	0.41
1:B:63:PHE:HE1	1:B:68:ILE:HD11	1.86	0.41
1:B:350:LEU:O	1:B:354:GLU:HG3	2.21	0.41
1:A:181:PRO:C	1:A:183:ASP:H	2.29	0.41
1:A:276:ARG:HE	1:A:278:ILE:CD1	2.35	0.40
1:B:148:ILE:CD1	1:B:161:LEU:HD21	2.51	0.40
1:A:173:ILE:HA	1:A:176:ILE:HD12	2.04	0.40
1:A:266:ARG:HD2	1:B:155:GLU:OE1	2.21	0.40

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	371/376 (99%)	360 (97%)	10 (3%)	1 (0%)	36	35
1	B	372/376 (99%)	363 (98%)	8 (2%)	1 (0%)	36	35
All	All	743/752 (99%)	723 (97%)	18 (2%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	HIS

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Mol	Chain	Res	Type
1	B	66	SER

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	323/326 (99%)	303 (94%)	20 (6%)	16	13
1	B	324/326 (99%)	308 (95%)	16 (5%)	22	20
All	All	647/652 (99%)	611 (94%)	36 (6%)	19	16

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	48	LYS
1	A	49	GLU
1	A	57	ILE
1	A	58	THR
1	A	62	GLU
1	A	64	GLU
1	A	65	ASP
1	A	68	ILE
1	A	128	LYS
1	A	157	GLU
1	A	172	LYS
1	A	185	LEU
1	A	186	LYS
1	A	200	SER
1	A	231	GLU
1	A	276	ARG
1	A	278	ILE
1	A	281	SER
1	A	297	LYS
1	B	31	LEU
1	B	45	LYS

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Mol	Chain	Res	Type
1	B	49	GLU
1	B	64	GLU
1	B	78	GLU
1	B	85	LYS
1	B	133	GLU
1	B	136	THR
1	B	139	ILE
1	B	158	LYS
1	B	175	LYS
1	B	187	HIS
1	B	191	ASN
1	B	275	LEU
1	B	278	ILE
1	B	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	69	ASN
1	A	244	ASN
1	A	310	ASN
1	A	331	HIS
1	A	357	HIS
1	B	18	GLN
1	B	54	ASN
1	B	69	ASN
1	B	108	HIS
1	B	244	ASN
1	B	331	HIS
1	B	342	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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$
3	FOM	B	901	-	4,4,10	1.65	1 (25%)	6,6,13	0.72	0
2	NDP	A	3001	-	51,52,52	1.33	7 (13%)	71,80,80	1.46	9 (12%)
2	NDP	A	3003	-	29,29,52	1.22	5 (17%)	44,45,80	1.78	12 (27%)
3	FOM	A	900	-	4,4,10	1.95	2 (50%)	6,6,13	1.28	1 (16%)
2	NDP	B	3002	-	51,52,52	1.63	11 (21%)	71,80,80	1.49	8 (11%)

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	3001	-	-	5/34/77/77	0/5/5/5
2	NDP	A	3003	-	-	4/15/31/77	0/3/3/5
2	NDP	B	3002	-	-	8/34/77/77	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NDP	PN-O3	4.77	1.64	1.59
2	B	3002	NDP	P2B-O2B	3.75	1.66	1.59
2	B	3002	NDP	PA-O3	3.33	1.63	1.59
2	A	3001	NDP	C4N-C5N	-3.26	1.40	1.49
2	B	3002	NDP	C4N-C5N	-3.24	1.40	1.49
2	B	3002	NDP	C5A-N7A	-3.10	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NDP	O4D-C1D	3.02	1.49	1.42
2	A	3001	NDP	PA-O3	2.99	1.62	1.59
2	A	3001	NDP	C4N-C3N	2.90	1.55	1.50
2	A	3003	NDP	C5A-N7A	-2.85	1.33	1.39
2	A	3001	NDP	P2B-O2B	2.73	1.64	1.59
2	B	3002	NDP	C4N-C3N	2.66	1.55	1.50
2	A	3001	NDP	C5A-N7A	-2.58	1.34	1.39
3	A	900	FOM	PA1-OP3	2.46	1.61	1.54
2	B	3002	NDP	C6N-C5N	2.45	1.40	1.33
2	A	3001	NDP	C6N-C5N	2.42	1.40	1.33
2	B	3002	NDP	C7N-C3N	2.42	1.53	1.48
3	A	900	FOM	PA1-OP2	2.40	1.61	1.54
2	B	3002	NDP	C4A-N9A	-2.32	1.32	1.37
2	A	3003	NDP	PA-O3	2.32	1.63	1.54
2	A	3003	NDP	PA-O2A	2.29	1.63	1.54
2	B	3002	NDP	PA-O2A	2.26	1.65	1.55
2	A	3001	NDP	PN-O3	2.18	1.61	1.59
2	A	3003	NDP	C8A-N9A	-2.09	1.34	1.37
3	B	901	FOM	PA1-C4	2.03	1.82	1.77
2	A	3003	NDP	C4A-N9A	-2.01	1.33	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NDP	N3A-C2A-N1A	-5.32	120.53	128.58
2	B	3002	NDP	N3A-C2A-N1A	-5.14	120.80	128.58
2	A	3003	NDP	N3A-C2A-N1A	-4.95	121.09	128.58
2	A	3001	NDP	C5A-C4A-N3A	-4.55	120.45	126.72
2	B	3002	NDP	C5A-C4A-N3A	-4.49	120.54	126.72
2	A	3003	NDP	C5A-C4A-N3A	-4.27	120.83	126.72
2	A	3001	NDP	N3A-C4A-N9A	3.65	133.37	127.17
2	B	3002	NDP	N9A-C8A-N7A	-3.63	108.79	113.94
2	A	3003	NDP	C2B-C1B-N9A	-3.62	107.79	113.75
2	B	3002	NDP	N3A-C4A-N9A	3.52	133.15	127.17
2	A	3001	NDP	C2A-N3A-C4A	3.38	120.09	111.83
2	B	3002	NDP	C2A-N3A-C4A	3.34	119.99	111.83
2	A	3003	NDP	N3A-C4A-N9A	3.27	132.72	127.17
2	A	3001	NDP	N9A-C8A-N7A	-3.11	109.53	113.94
2	A	3003	NDP	C2A-N3A-C4A	2.99	119.12	111.83
2	A	3003	NDP	N9A-C8A-N7A	-2.92	109.79	113.94
2	B	3002	NDP	C4A-N9A-C8A	2.91	108.80	105.74
2	A	3001	NDP	C4A-N9A-C8A	2.82	108.69	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3003	NDP	O5B-PA-O1A	2.73	113.82	106.44
3	A	900	FOM	OP3-PA1-OP2	-2.61	100.91	108.22
2	A	3003	NDP	C4A-N9A-C8A	2.58	108.45	105.74
2	B	3002	NDP	O4D-C1D-N1N	2.50	112.86	108.08
2	B	3002	NDP	C5A-N7A-C8A	2.42	107.26	103.45
2	A	3001	NDP	C3N-C2N-N1N	-2.41	119.67	123.20
2	A	3003	NDP	C2A-N1A-C6A	2.39	122.66	118.73
2	A	3003	NDP	O4B-C1B-N9A	2.39	112.68	108.09
2	A	3003	NDP	C5A-N7A-C8A	2.27	107.02	103.45
2	A	3001	NDP	C5A-N7A-C8A	2.19	106.89	103.45
2	A	3001	NDP	O3B-C3B-C2B	-2.03	105.50	111.19
2	A	3003	NDP	C4A-C5A-N7A	-2.01	108.29	110.58

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3003	NDP	C5B-O5B-PA-O3
2	B	3002	NDP	C5B-O5B-PA-O1A
2	A	3003	NDP	O4B-C4B-C5B-O5B
2	A	3001	NDP	O4B-C4B-C5B-O5B
2	B	3002	NDP	O4B-C4B-C5B-O5B
2	A	3001	NDP	C2B-C1B-N9A-C8A
2	A	3001	NDP	O4D-C1D-N1N-C6N
2	A	3001	NDP	C5B-O5B-PA-O1A
2	A	3003	NDP	C5B-O5B-PA-O1A
2	A	3003	NDP	C3B-C4B-C5B-O5B
2	B	3002	NDP	C2B-C1B-N9A-C8A
2	B	3002	NDP	O4D-C1D-N1N-C6N
2	A	3001	NDP	C2N-C3N-C7N-N7N
2	B	3002	NDP	O4D-C4D-C5D-O5D
2	B	3002	NDP	C2N-C3N-C7N-N7N
2	B	3002	NDP	PN-O3-PA-O1A
2	B	3002	NDP	C2B-O2B-P2B-O3X

There are no ring outliers.

3 monomers are involved in 7 short contacts:

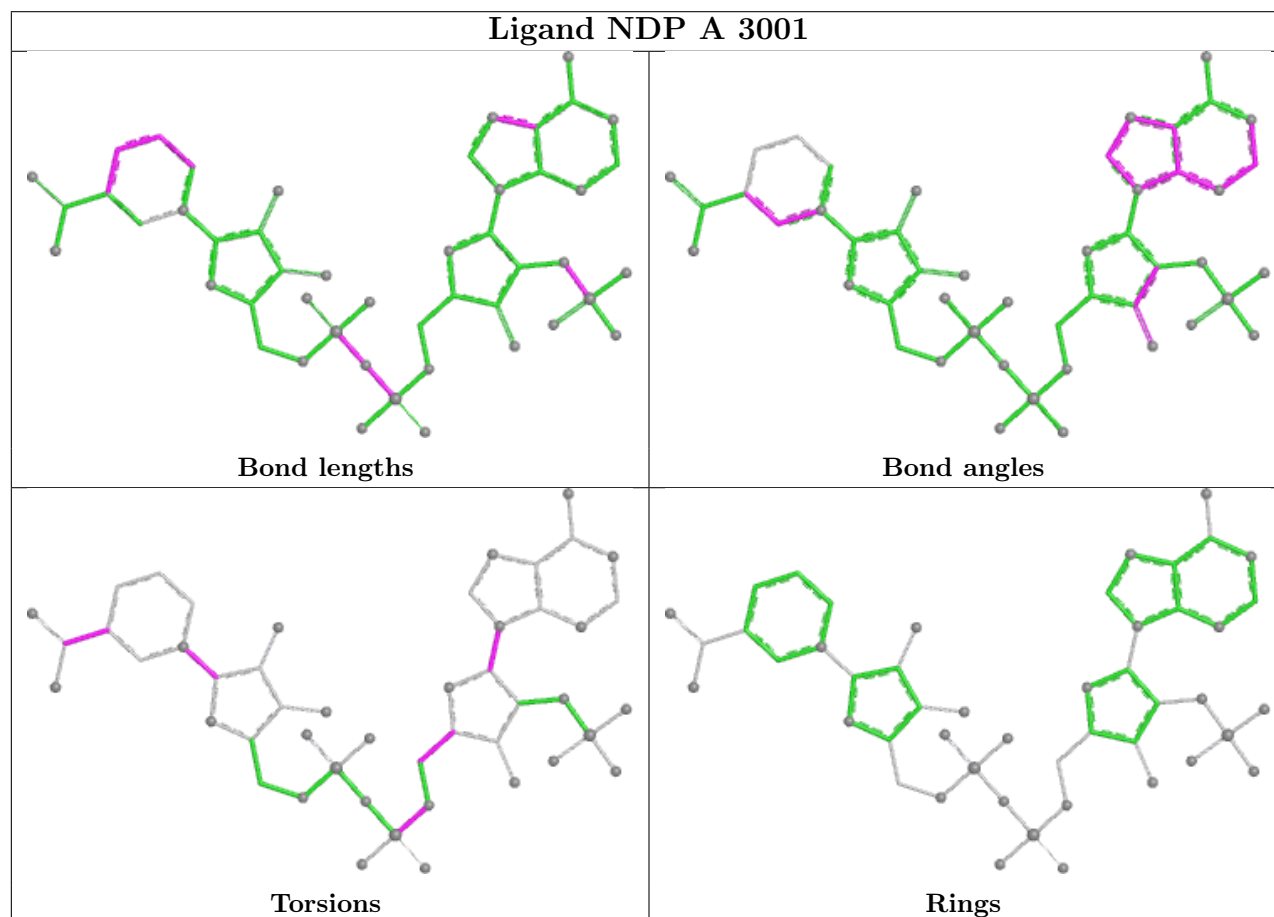
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	NDP	2	0
3	A	900	FOM	4	0

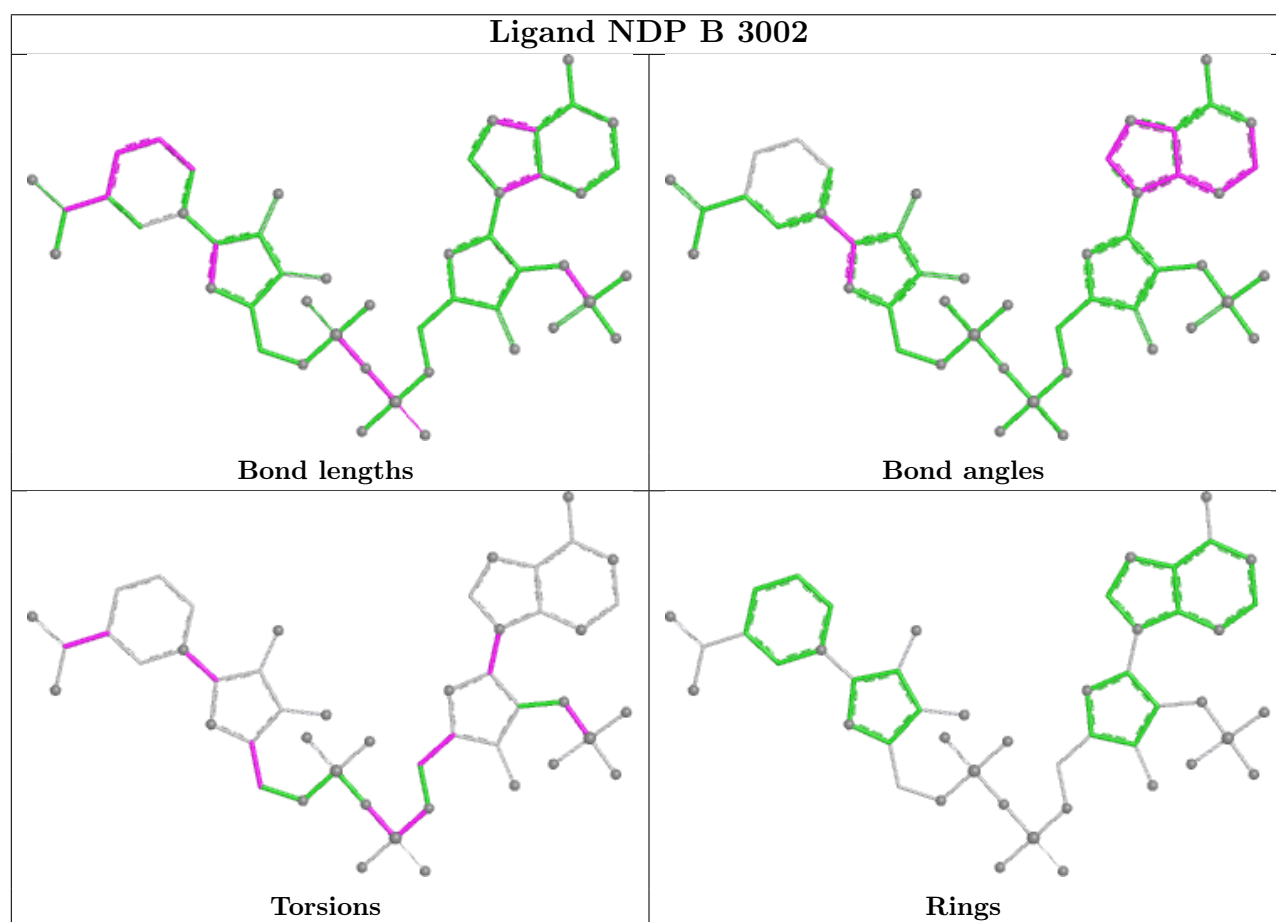
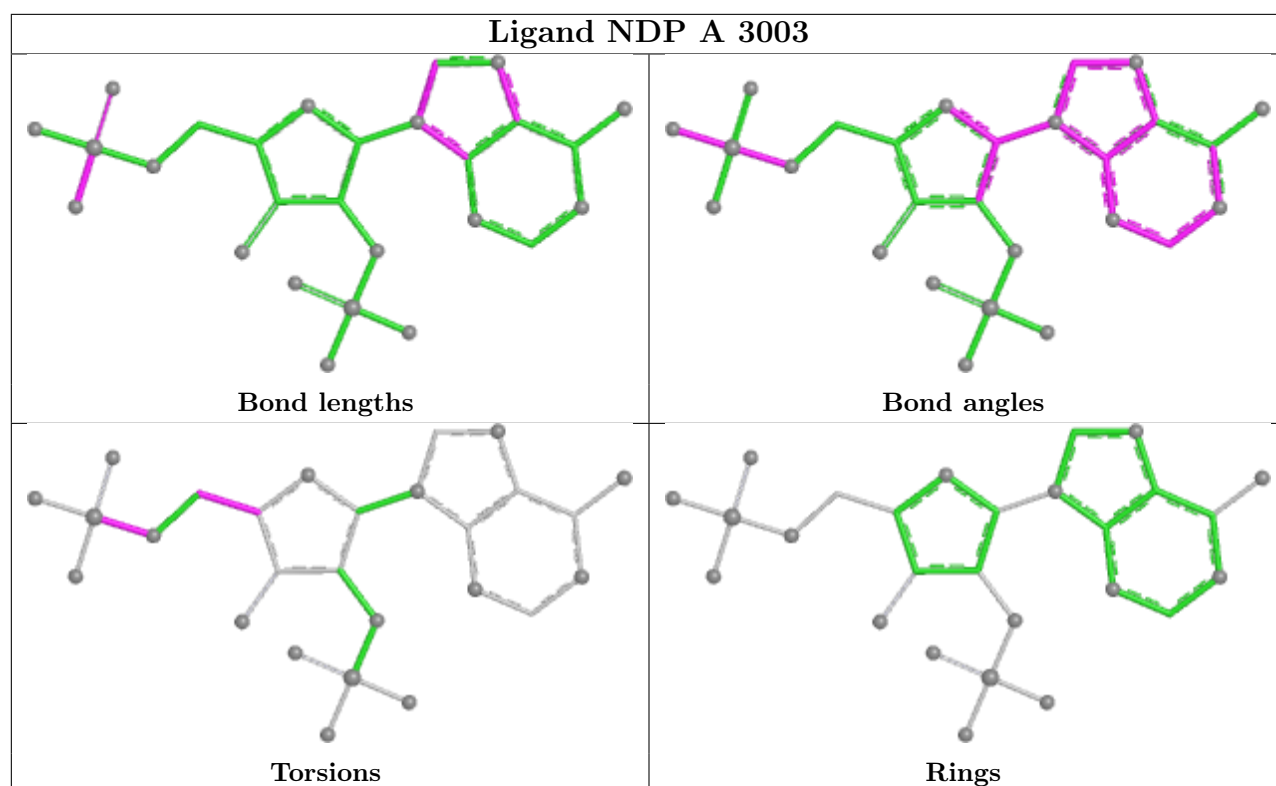
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	NDP	1	0

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	370/376 (98%)	0.81	41 (11%) 10 9	29, 47, 71, 84	14 (3%)
1	B	373/376 (99%)	0.68	25 (6%) 24 22	28, 48, 66, 82	6 (1%)
All	All	743/752 (98%)	0.74	66 (8%) 15 14	28, 48, 69, 84	20 (2%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	VAL	13.7
1	A	185	LEU	11.8
1	A	184	VAL	11.3
1	B	190	TRP	10.4
1	B	188	PRO	9.1
1	A	190	TRP	8.7
1	A	188	PRO	8.7
1	B	187	HIS	7.9
1	B	189	VAL	7.6
1	A	187	HIS	7.1
1	A	183	ASP	6.8
1	A	191	ASN	6.5
1	B	191	ASN	5.7
1	A	192	MET	4.8
1	B	374	THR	4.6
1	A	182	GLU	4.5
1	B	185	LEU	4.0
1	B	63	PHE	4.0
1	B	65	ASP	3.5
1	A	186	LYS	3.5
1	B	344	TYR	3.3
1	B	275	LEU	3.2
1	A	212	GLU	3.1
1	A	167	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	44	PHE	3.0
1	A	274	PHE	3.0
1	A	278	ILE	2.9
1	A	275	LEU	2.9
1	B	49	GLU	2.7
1	B	192	MET	2.7
1	A	196	ILE	2.7
1	A	351	ASP	2.6
1	A	200	SER	2.6
1	A	173	ILE	2.6
1	A	225	GLU	2.6
1	A	370	TRP	2.6
1	A	277	THR	2.5
1	A	133	GLU	2.5
1	A	61	VAL	2.5
1	B	278	ILE	2.5
1	B	358	PHE	2.5
1	A	49	GLU	2.4
1	A	354	GLU	2.4
1	A	171	TRP	2.4
1	A	372	SER	2.3
1	A	155	GLU	2.3
1	B	66	SER	2.3
1	B	61	VAL	2.3
1	B	133	GLU	2.3
1	B	274	PHE	2.3
1	A	283	GLU	2.2
1	B	301	ASP	2.2
1	A	194	ALA	2.2
1	B	43	ALA	2.2
1	A	138	LEU	2.2
1	A	181	PRO	2.2
1	A	74	SER	2.2
1	A	60	ASP	2.2
1	A	168	LEU	2.1
1	B	339	GLU	2.1
1	B	369	GLU	2.1
1	B	44	PHE	2.1
1	A	29	ILE	2.0
1	A	63	PHE	2.0
1	B	370	TRP	2.0
1	A	276	ARG	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 [i](#)

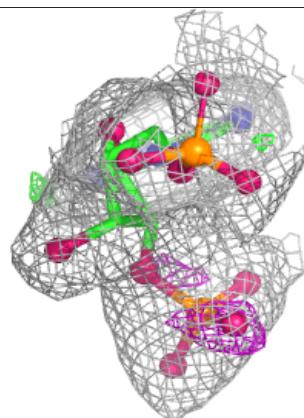
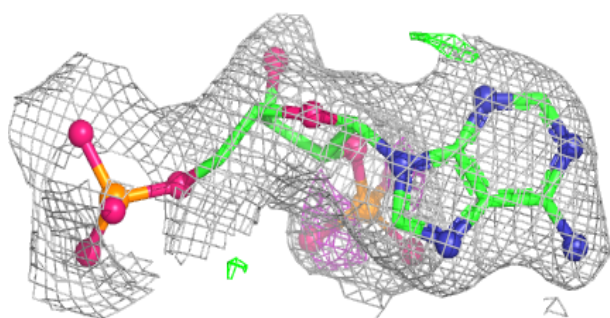
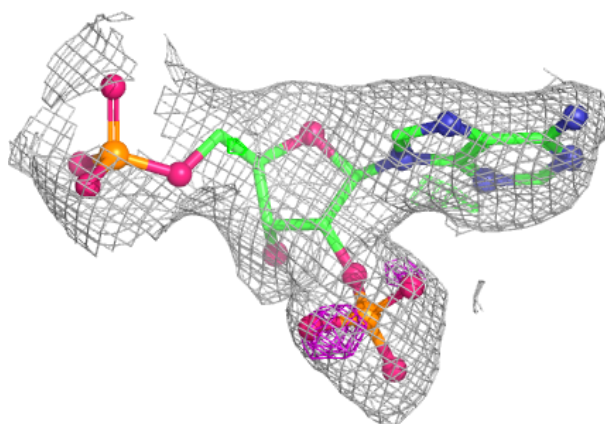
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	MG	B	501	1/1	0.82	0.10	52,52,52,52	1
3	FOM	B	901	5/11	0.83	0.22	52,52,53,53	5
2	NDP	A	3003	27/48	0.88	0.10	49,56,78,79	0
3	FOM	A	900	5/11	0.89	0.12	56,57,58,59	0
2	NDP	B	3002	48/48	0.90	0.10	49,59,67,68	0
2	NDP	A	3001	48/48	0.92	0.10	44,54,58,60	0
4	MG	A	500	1/1	0.94	0.14	53,53,53,53	0

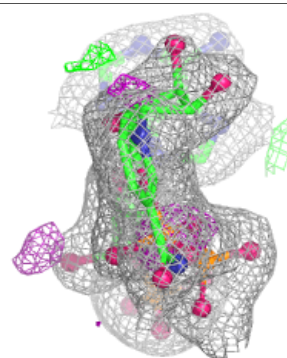
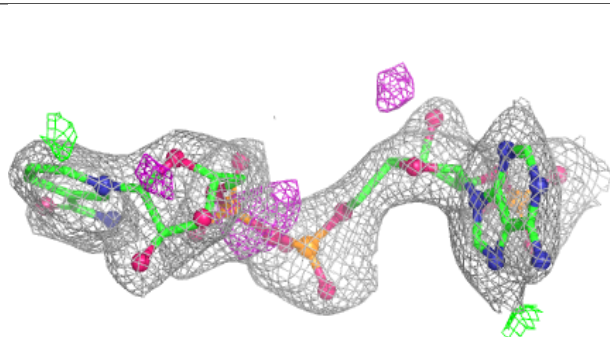
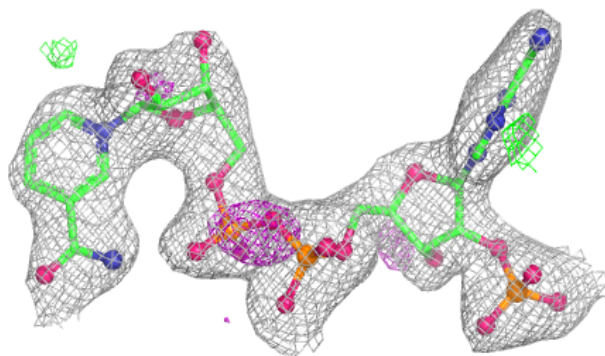
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP A 3003:

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

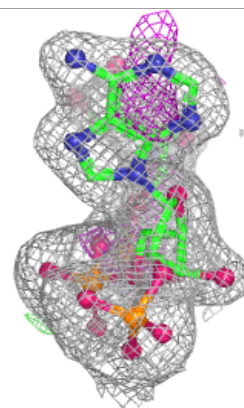
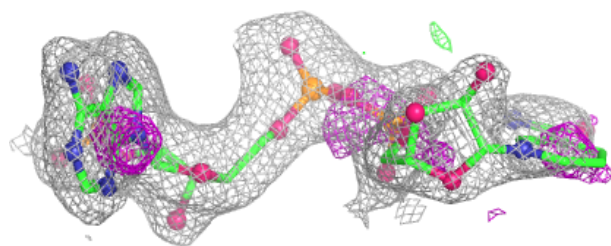
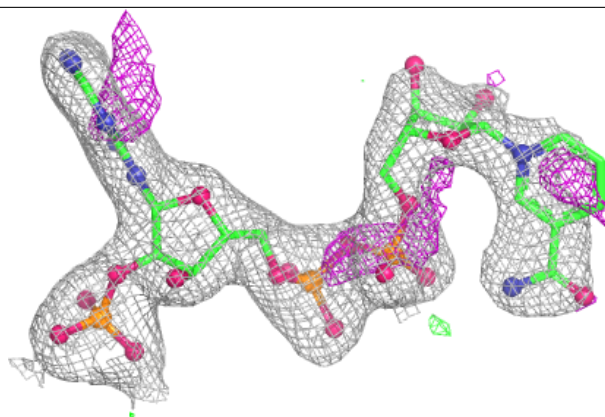
**Electron density around NDP B 3002:**

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



Electron density around NDP A 3001:

$2mF_o-DF_c$ (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.