



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:40 AM UTC

PDB ID : 3WG6 / pdb_00003wg6
Title : Crystal structure of conjugated polyketone reductase C1 from *Candida parapsilosis* complexed with NADPH
Authors : Qin, H.-M.; Yamamura, A.; Miyakawa, T.; Maruoka, S.; Ohtsuka, J.; Nagata, K.; Kataoka, M.; Shimizu, S.; Tanokura, M.
Deposited on : 2013-07-28
Resolution : 2.20 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

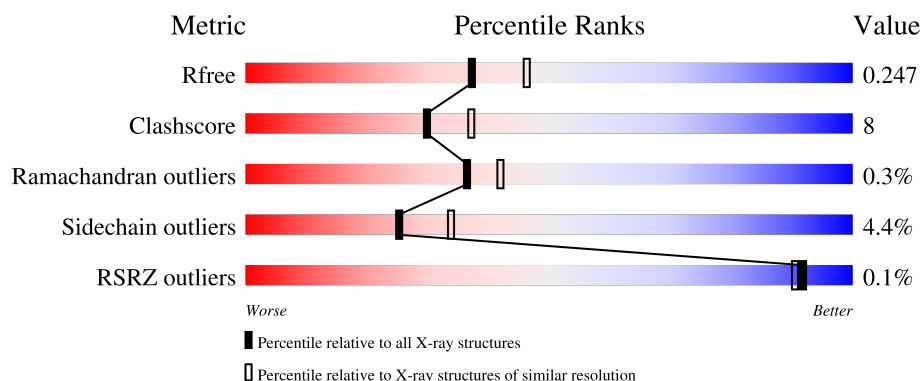
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	307	 77% 17% . . .
1	B	307	 79% 15% . .
1	C	307	 81% 16% .
1	D	307	 77% 19% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10104 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 Conjugated polyketone reductase C1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	0	0	0
			2408	1532	412	464			
1	B	295	Total	C	N	O	0	0	0
			2378	1516	405	457			
1	C	298	Total	C	N	O	0	0	0
			2400	1528	411	461			
1	D	298	Total	C	N	O	0	0	0
			2400	1528	411	461			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q76L37
A	-1	SER	-	expression tag	UNP Q76L37
A	0	HIS	-	expression tag	UNP Q76L37
B	-2	GLY	-	expression tag	UNP Q76L37
B	-1	SER	-	expression tag	UNP Q76L37
B	0	HIS	-	expression tag	UNP Q76L37
C	-2	GLY	-	expression tag	UNP Q76L37
C	-1	SER	-	expression tag	UNP Q76L37
C	0	HIS	-	expression tag	UNP Q76L37
D	-2	GLY	-	expression tag	UNP Q76L37
D	-1	SER	-	expression tag	UNP Q76L37
D	0	HIS	-	expression tag	UNP Q76L37

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

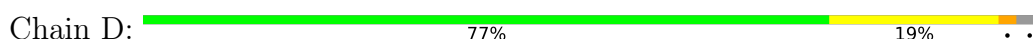


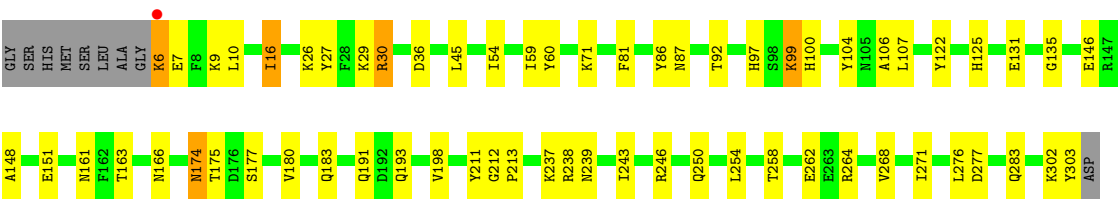
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	62	Total O 62 62	0	0
3	C	98	Total O 98 98	0	0
3	D	67	Total O 67 67	0	0

- Molecule 1: Conjugated polyketone reductase C1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.07Å 84.93Å 136.16Å 90.00° 96.17° 90.00°	Depositor
Resolution (Å)	19.78 – 2.20 19.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.78-2.20) 99.1 (19.78-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.182 , 0.242 0.189 , 0.247	Depositor DCC
R_{free} test set	3424 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10104	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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

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	1.23	2/2455 (0.1%)	1.20	8/3311 (0.2%)
1	B	1.16	0/2423	1.12	4/3266 (0.1%)
1	C	1.29	2/2447 (0.1%)	1.15	4/3300 (0.1%)
1	D	1.21	5/2447 (0.2%)	1.14	3/3300 (0.1%)
All	All	1.22	9/9772 (0.1%)	1.15	19/13177 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	148	ALA	CA-CB	6.09	1.62	1.53
1	D	54	ILE	N-CA	5.65	1.53	1.46
1	D	198	VAL	CA-CB	5.56	1.60	1.54
1	C	149	LYS	CE-NZ	5.54	1.66	1.49
1	A	178	ILE	CA-CB	-5.32	1.50	1.55
1	A	194	THR	CA-CB	5.28	1.60	1.53
1	D	258	THR	CA-CB	5.24	1.62	1.53
1	C	239	ASN	CB-CG	-5.18	1.39	1.52
1	D	59	ILE	CA-CB	5.17	1.60	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ILE	CA-C-N	-7.92	111.84	119.76
1	A	16	ILE	C-N-CA	-7.92	111.84	119.76
1	C	178	ILE	CA-C-N	-7.69	112.09	119.85
1	C	178	ILE	C-N-CA	-7.69	112.09	119.85
1	A	197	ILE	N-CA-C	6.29	117.04	110.62
1	A	257	THR	CB-CA-C	-6.15	99.71	112.44
1	A	85	LYS	CD-CE-NZ	6.03	131.19	111.90
1	A	238	ARG	CB-CG-CD	5.98	125.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	LYS	N-CA-C	-5.97	104.85	111.36
1	C	239	ASN	CB-CA-C	-5.73	99.50	109.64
1	D	16	ILE	CA-C-N	-5.49	114.27	119.76
1	D	16	ILE	C-N-CA	-5.49	114.27	119.76
1	C	176	ASP	N-CA-C	5.39	120.01	113.38
1	B	215	GLY	CA-C-N	-5.39	114.06	119.56
1	B	215	GLY	C-N-CA	-5.39	114.06	119.56
1	A	223	GLY	CA-C-N	5.09	124.75	119.56
1	A	223	GLY	C-N-CA	5.09	124.75	119.56
1	D	27	TYR	N-CA-C	5.09	119.49	113.28
1	B	252	GLY	N-CA-C	-5.08	107.80	115.32

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	2408	0	2395	54	0
1	B	2378	0	2374	35	0
1	C	2400	0	2391	32	0
1	D	2400	0	2391	43	0
2	A	48	0	26	6	0
2	B	48	0	26	4	0
2	C	48	0	26	4	0
2	D	48	0	26	6	0
3	A	99	0	0	3	0
3	B	62	0	0	2	0
3	C	98	0	0	2	0
3	D	67	0	0	2	0
All	All	10104	0	9655	165	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 8.

All (165) 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:37:LYS:HB2	1:A:37:LYS:NZ	1.34	1.24
1:A:37:LYS:NZ	1:A:37:LYS:CB	2.05	1.17
1:A:37:LYS:CB	1:A:37:LYS:HZ3	1.58	1.17
1:D:6:LYS:HG2	1:D:7:GLU:H	1.13	1.06
1:A:37:LYS:HB2	1:A:37:LYS:HZ2	1.26	0.95
1:B:247:TRP:HE1	1:B:285:THR:HG22	1.30	0.95
1:D:246:ARG:HE	1:D:250:GLN:HE21	0.95	0.93
1:B:246:ARG:HE	1:B:250:GLN:HE21	0.91	0.91
1:D:174:ASN:C	1:D:174:ASN:HD22	1.87	0.82
1:C:97:HIS:HD2	3:C:3131:HOH:O	1.62	0.82
1:A:131:GLU:HG3	3:A:3177:HOH:O	1.80	0.81
1:D:246:ARG:HE	1:D:250:GLN:NE2	1.77	0.81
1:A:85:LYS:HD3	1:A:123:LEU:HD12	1.63	0.81
1:A:257:THR:HG23	2:A:3001:NDP:O2A	1.81	0.80
1:B:238:ARG:HG2	1:B:238:ARG:HH11	1.44	0.80
1:B:246:ARG:HE	1:B:250:GLN:NE2	1.77	0.79
1:D:246:ARG:NE	1:D:250:GLN:HE21	1.78	0.78
1:A:246:ARG:HE	1:A:250:GLN:HE21	1.30	0.78
1:B:246:ARG:NE	1:B:250:GLN:HE21	1.77	0.78
1:D:6:LYS:CG	1:D:7:GLU:H	1.97	0.77
1:D:6:LYS:HG2	1:D:7:GLU:N	1.93	0.76
1:A:37:LYS:HB2	1:A:37:LYS:HZ3	0.94	0.76
1:A:161:ASN:HD22	1:A:193:GLN:HE22	1.33	0.75
1:B:247:TRP:NE1	1:B:285:THR:HG22	2.01	0.75
1:B:161:ASN:HD22	1:B:193:GLN:HE22	1.37	0.73
1:B:250:GLN:HE22	1:B:276:LEU:H	1.34	0.71
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.55	0.71
3:B:3150:HOH:O	1:C:227:LYS:HD3	1.91	0.71
1:C:161:ASN:HD22	1:C:193:GLN:HE22	1.37	0.70
1:C:125:HIS:HD2	3:C:3114:HOH:O	1.75	0.70
1:B:285:THR:HG21	3:B:3109:HOH:O	1.91	0.69
1:C:183:GLN:NE2	2:C:3001:NDP:H71N	1.89	0.69
1:C:146:GLU:OE1	1:C:175:THR:HB	1.93	0.69
1:D:161:ASN:HD22	1:D:193:GLN:HE22	1.39	0.69
1:A:163:THR:H	1:A:166:ASN:HD22	1.38	0.68
1:C:211:TYR:CE1	2:C:3001:NDP:H41N	2.30	0.66
2:B:3001:NDP:H3D	2:B:3001:NDP:H6N	1.79	0.65
1:A:178:ILE:HD11	3:A:3139:HOH:O	1.96	0.65
1:A:257:THR:CG2	2:A:3001:NDP:O2A	2.45	0.64
1:B:247:TRP:HE1	1:B:285:THR:CG2	2.09	0.64
1:C:183:GLN:HE21	2:C:3001:NDP:H71N	1.46	0.64
1:A:217:ILE:HD13	1:A:244:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ARG:HH11	1:B:238:ARG:CG	2.11	0.63
1:A:102:ASN:ND2	1:A:105:ASN:H	1.97	0.63
1:A:217:ILE:HD11	1:A:229:LEU:HD13	1.81	0.63
1:D:183:GLN:HE21	2:D:3001:NDP:H71N	1.45	0.63
1:D:146:GLU:OE2	1:D:177:SER:HB2	1.99	0.63
1:A:133:SER:OG	1:A:134:HIS:HD2	1.80	0.62
1:D:163:THR:H	1:D:166:ASN:HD22	1.48	0.62
1:D:174:ASN:C	1:D:174:ASN:ND2	2.58	0.62
1:D:29:LYS:HB2	1:D:60:TYR:O	2.00	0.62
1:B:146:GLU:OE2	1:B:175:THR:HG22	2.00	0.61
1:D:183:GLN:NE2	2:D:3001:NDP:H71N	1.98	0.61
1:C:161:ASN:ND2	1:C:193:GLN:HE22	1.99	0.61
1:C:32:HIS:HD2	1:C:34:ASP:H	1.49	0.61
1:A:247:TRP:HE1	1:A:285:THR:HG22	1.65	0.60
1:D:250:GLN:HE22	1:D:276:LEU:H	1.48	0.60
1:A:247:TRP:HE1	1:A:285:THR:CG2	2.15	0.59
1:A:250:GLN:HE22	1:A:276:LEU:H	1.48	0.59
1:A:88:SER:O	1:A:134:HIS:HE1	1.86	0.58
1:D:161:ASN:ND2	1:D:193:GLN:HE22	2.01	0.58
1:B:161:ASN:ND2	1:B:193:GLN:HE22	2.01	0.58
1:B:281:GLU:O	1:B:285:THR:HG23	2.03	0.57
1:C:183:GLN:NE2	2:C:3001:NDP:H2N	2.19	0.57
1:C:212:GLY:N	1:C:213:PRO:CD	2.67	0.57
1:D:87:ASN:O	1:D:97:HIS:HB2	2.05	0.57
1:A:211:TYR:CE1	2:A:3001:NDP:H41N	2.40	0.56
1:C:163:THR:H	1:C:166:ASN:HD22	1.53	0.56
1:A:133:SER:OG	1:A:134:HIS:CD2	2.58	0.56
1:A:161:ASN:ND2	1:A:193:GLN:HE22	2.02	0.56
1:B:211:TYR:CE1	2:B:3001:NDP:H41N	2.42	0.55
1:B:142:TRP:CD1	1:B:175:THR:HG21	2.41	0.55
1:A:250:GLN:NE2	1:A:276:LEU:H	2.05	0.55
1:C:117:GLU:HG2	1:C:118:TYR:HD2	1.71	0.55
1:D:212:GLY:N	1:D:213:PRO:CD	2.69	0.55
1:A:292:THR:HG21	1:A:304:ASP:HB3	1.88	0.55
1:A:247:TRP:NE1	1:A:285:THR:HG22	2.22	0.55
1:B:264:ARG:HA	1:B:267:ASP:HB2	1.89	0.55
1:D:264:ARG:NH1	2:D:3001:NDP:O2X	2.41	0.54
1:D:99:LYS:HG2	3:D:3114:HOH:O	2.06	0.54
1:B:30:ARG:HH11	1:B:30:ARG:CG	2.21	0.53
1:D:131:GLU:O	1:D:135:GLY:N	2.36	0.53
1:A:37:LYS:HZ3	1:A:37:LYS:HB3	1.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:NH1	3:A:3190:HOH:O	2.41	0.52
1:A:235:LYS:HE3	1:A:280:ASP:OD2	2.09	0.52
1:A:212:GLY:N	1:A:213:PRO:CD	2.72	0.52
1:A:247:TRP:CZ2	1:A:285:THR:HG22	2.44	0.52
1:A:183:GLN:NE2	2:A:3001:NDP:H2N	2.25	0.52
1:B:296:PHE:O	1:B:297:SER:C	2.52	0.52
1:A:281:GLU:O	1:A:285:THR:HG23	2.11	0.51
1:D:45:LEU:HD21	1:D:262:GLU:HG3	1.92	0.51
1:A:217:ILE:CD1	1:A:229:LEU:HD13	2.40	0.51
1:D:86:TYR:O	1:D:125:HIS:HB2	2.11	0.50
1:B:146:GLU:OE2	1:B:175:THR:CG2	2.59	0.50
1:C:163:THR:H	1:C:166:ASN:ND2	2.09	0.49
1:B:91:HIS:HA	1:B:128:TYR:CG	2.48	0.49
1:D:104:TYR:OH	1:D:151:GLU:OE1	2.31	0.49
1:A:102:ASN:HD22	1:A:102:ASN:C	2.21	0.49
1:D:163:THR:H	1:D:166:ASN:ND2	2.11	0.48
1:D:211:TYR:CE1	2:D:3001:NDP:H41N	2.48	0.48
1:D:6:LYS:CG	1:D:7:GLU:N	2.65	0.48
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.79	0.48
1:C:107:LEU:HD22	1:C:122:TYR:CD2	2.48	0.48
2:D:3001:NDP:H6N	2:D:3001:NDP:H3D	1.94	0.48
1:C:162:PHE:CD2	1:C:166:ASN:HB3	2.49	0.48
1:B:146:GLU:OE1	1:B:175:THR:HG23	2.13	0.48
1:A:163:THR:HG22	1:A:194:THR:HG21	1.96	0.48
1:B:163:THR:HG22	1:B:194:THR:HG21	1.97	0.47
1:A:20:ALA:HB2	1:A:53:HIS:CE1	2.51	0.46
1:B:168:LYS:HB3	1:B:168:LYS:HE3	1.66	0.46
1:A:237:LYS:O	1:A:238:ARG:HD2	2.15	0.46
1:B:58:GLU:HB2	1:B:85:LYS:O	2.16	0.46
1:A:183:GLN:NE2	2:A:3001:NDP:H71N	2.14	0.46
1:C:55:ASP:OD2	1:C:85:LYS:NZ	2.46	0.46
1:A:228:VAL:O	1:A:232:LEU:HG	2.15	0.45
1:D:237:LYS:O	1:D:238:ARG:HD3	2.17	0.45
1:D:268:VAL:O	1:D:271:ILE:HG12	2.17	0.45
1:C:201:SER:CB	1:C:208:ILE:HD11	2.46	0.45
1:B:261:LYS:HE2	2:B:3001:NDP:O1X	2.17	0.45
1:B:24:GLY:O	1:B:25:THR:C	2.60	0.45
1:C:162:PHE:H	1:C:182:ASN:HD21	1.65	0.45
1:B:136:PHE:HB2	1:B:140:GLU:HB3	1.97	0.45
1:C:104:TYR:CE2	1:C:108:LYS:HE3	2.52	0.45
1:A:91:HIS:HA	1:A:128:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:TYR:C	1:A:213:PRO:HD3	2.42	0.45
2:B:3001:NDP:H6N	2:B:3001:NDP:C3D	2.47	0.45
1:B:195:PRO:HG2	1:D:303:TYR:HE1	1.82	0.44
1:B:211:TYR:C	1:B:213:PRO:HD3	2.42	0.44
1:C:97:HIS:O	1:C:98:SER:C	2.60	0.44
1:A:217:ILE:HG13	1:A:221:ARG:NH1	2.33	0.44
1:A:171:LEU:HD13	1:A:204:GLN:HE21	1.82	0.44
1:D:36:ASP:OD1	1:D:36:ASP:C	2.60	0.44
1:D:277:ASP:OD1	1:D:277:ASP:C	2.60	0.44
1:B:238:ARG:CG	1:B:238:ARG:NH1	2.74	0.44
1:A:151:GLU:HG2	1:A:153:LEU:HG	2.00	0.44
1:C:30:ARG:HD2	1:D:92:THR:HB	2.00	0.44
1:A:88:SER:O	1:A:134:HIS:CE1	2.69	0.43
1:D:10:LEU:HD22	1:D:180:VAL:HB	2.00	0.43
1:D:100:HIS:CD2	1:D:106:ALA:HA	2.53	0.43
1:C:86:TYR:O	1:C:125:HIS:HB2	2.18	0.43
1:A:247:TRP:CE2	1:A:285:THR:HG22	2.54	0.43
1:D:254:LEU:C	1:D:254:LEU:HD23	2.43	0.43
1:C:80:VAL:HG12	1:C:81:PHE:N	2.33	0.43
1:A:37:LYS:CB	1:A:37:LYS:HZ2	1.97	0.43
1:C:211:TYR:C	1:C:213:PRO:HD3	2.44	0.42
2:A:3001:NDP:H6N	2:A:3001:NDP:H3D	2.01	0.42
1:B:147:ARG:O	1:B:151:GLU:HG3	2.19	0.42
1:D:174:ASN:HB2	3:D:3155:HOH:O	2.19	0.42
1:C:214:LEU:O	1:C:215:GLY:C	2.63	0.42
1:B:146:GLU:CD	1:B:175:THR:CG2	2.93	0.42
1:D:16:ILE:HG13	1:D:81:PHE:CZ	2.54	0.42
1:D:183:GLN:NE2	2:D:3001:NDP:H2N	2.33	0.41
1:A:18:ALA:O	1:A:255:PRO:HD2	2.20	0.41
1:A:215:GLY:N	1:A:216:PRO:CD	2.83	0.41
1:D:107:LEU:HB2	1:D:122:TYR:CZ	2.55	0.41
1:A:155:ARG:NH1	1:A:155:ARG:HG2	2.36	0.41
1:A:137:ASP:C	1:A:137:ASP:OD2	2.64	0.41
1:D:239:ASN:O	1:D:243:ILE:HG12	2.21	0.41
1:C:20:ALA:HB2	1:C:53:HIS:CE1	2.56	0.40
1:D:250:GLN:NE2	1:D:276:LEU:H	2.16	0.40
1:C:92:THR:HB	1:D:30:ARG:HD3	2.04	0.40
1:C:39:LEU:O	1:C:40:ILE:C	2.63	0.40
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.96	0.40
1:B:86:TYR:HB2	1:B:122:TYR:OH	2.22	0.40
1:C:162:PHE:HA	1:C:166:ASN:HD22	1.86	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	297/307 (97%)	287 (97%)	9 (3%)	1 (0%)	36	42
1	B	291/307 (95%)	279 (96%)	9 (3%)	3 (1%)	12	11
1	C	296/307 (96%)	284 (96%)	12 (4%)	0	100	100
1	D	296/307 (96%)	283 (96%)	13 (4%)	0	100	100
All	All	1180/1228 (96%)	1133 (96%)	43 (4%)	4 (0%)	36	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	THR
1	B	97	HIS
1	A	25	THR
1	B	26	LYS

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	261/266 (98%)	248 (95%)	13 (5%)	22	28
1	B	258/266 (97%)	243 (94%)	15 (6%)	18	22
1	C	260/266 (98%)	253 (97%)	7 (3%)	39	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	260/266 (98%)	249 (96%)	11 (4%)	26	36
All	All	1039/1064 (98%)	993 (96%)	46 (4%)	25	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	28	PHE
1	A	37	LYS
1	A	71	LYS
1	A	80	VAL
1	A	85	LYS
1	A	102	ASN
1	A	195	PRO
1	A	217	ILE
1	A	221	ARG
1	A	234	GLU
1	A	238	ARG
1	A	257	THR
1	B	9	LYS
1	B	26	LYS
1	B	30	ARG
1	B	70	LEU
1	B	149	LYS
1	B	168	LYS
1	B	178	ILE
1	B	221	ARG
1	B	230	SER
1	B	237	LYS
1	B	238	ARG
1	B	243	ILE
1	B	275	GLU
1	B	285	THR
1	B	298	LYS
1	C	38	GLN
1	C	49	SER
1	C	108	LYS
1	C	225	LEU
1	C	234	GLU
1	C	258	THR
1	C	302	LYS
1	D	6	LYS

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Mol	Chain	Res	Type
1	D	9	LYS
1	D	26	LYS
1	D	30	ARG
1	D	71	LYS
1	D	99	LYS
1	D	174	ASN
1	D	175	THR
1	D	191	GLN
1	D	283	GLN
1	D	302	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	102	ASN
1	A	105	ASN
1	A	134	HIS
1	A	161	ASN
1	A	166	ASN
1	A	182	ASN
1	A	183	GLN
1	A	191	GLN
1	A	250	GLN
1	B	100	HIS
1	B	161	ASN
1	B	204	GLN
1	B	219	GLN
1	B	250	GLN
1	B	266	ASN
1	C	32	HIS
1	C	63	ASN
1	C	91	HIS
1	C	97	HIS
1	C	100	HIS
1	C	125	HIS
1	C	150	ASN
1	C	161	ASN
1	C	166	ASN
1	C	182	ASN
1	C	183	GLN
1	C	202	GLN

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Mol	Chain	Res	Type
1	C	204	GLN
1	C	239	ASN
1	C	295	GLN
1	D	14	ASN
1	D	63	ASN
1	D	72	ASN
1	D	100	HIS
1	D	101	GLN
1	D	161	ASN
1	D	166	ASN
1	D	174	ASN
1	D	183	GLN
1	D	250	GLN
1	D	266	ASN

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](#)

4 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	C	3001	-	51,52,52	1.51	7 (13%)	71,80,80	1.68	14 (19%)
2	NDP	A	3001	-	51,52,52	1.53	5 (9%)	71,80,80	1.71	15 (21%)
2	NDP	D	3001	-	51,52,52	1.53	9 (17%)	71,80,80	1.76	22 (30%)
2	NDP	B	3001	-	51,52,52	1.69	9 (17%)	71,80,80	1.69	14 (19%)

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	C	3001	-	-	4/34/77/77	0/5/5/5
2	NDP	A	3001	-	-	3/34/77/77	0/5/5/5
2	NDP	D	3001	-	-	4/34/77/77	0/5/5/5
2	NDP	B	3001	-	-	4/34/77/77	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	NDP	O7N-C7N	6.96	1.40	1.24
2	A	3001	NDP	O7N-C7N	6.87	1.40	1.24
2	D	3001	NDP	O7N-C7N	5.62	1.37	1.24
2	C	3001	NDP	O7N-C7N	4.81	1.35	1.24
2	B	3001	NDP	PN-O3	4.69	1.64	1.59
2	C	3001	NDP	PN-O3	4.01	1.63	1.59
2	D	3001	NDP	PA-O3	3.69	1.63	1.59
2	B	3001	NDP	PA-O3	3.63	1.63	1.59
2	D	3001	NDP	C2A-N1A	3.34	1.39	1.33
2	C	3001	NDP	C2A-N1A	3.28	1.39	1.33
2	C	3001	NDP	C2A-N3A	3.24	1.39	1.33
2	A	3001	NDP	C2A-N3A	3.01	1.39	1.33
2	C	3001	NDP	PA-O3	2.99	1.62	1.59
2	B	3001	NDP	C2A-N1A	2.97	1.39	1.33
2	D	3001	NDP	C2A-N3A	2.71	1.38	1.33
2	D	3001	NDP	C5A-N7A	-2.69	1.34	1.39
2	D	3001	NDP	PN-O3	2.68	1.62	1.59
2	D	3001	NDP	C4A-N3A	2.67	1.39	1.34
2	A	3001	NDP	C4N-C3N	2.63	1.55	1.50
2	B	3001	NDP	C5A-N7A	-2.58	1.34	1.39
2	A	3001	NDP	C2A-N1A	2.46	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	NDP	C2A-N3A	2.45	1.38	1.33
2	C	3001	NDP	C5A-N7A	-2.35	1.34	1.39
2	D	3001	NDP	C8A-N7A	2.28	1.36	1.31
2	B	3001	NDP	O4B-C4B	-2.23	1.40	1.45
2	B	3001	NDP	C6N-C5N	2.18	1.39	1.33
2	C	3001	NDP	C6N-C5N	2.17	1.39	1.33
2	D	3001	NDP	PA-O2A	-2.12	1.45	1.55
2	A	3001	NDP	PN-O2N	-2.11	1.45	1.55
2	B	3001	NDP	C8A-N7A	2.03	1.35	1.31

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3001	NDP	N3A-C2A-N1A	-6.29	119.06	128.58
2	D	3001	NDP	N3A-C2A-N1A	-6.13	119.30	128.58
2	B	3001	NDP	N3A-C2A-N1A	-5.35	120.48	128.58
2	C	3001	NDP	N9A-C8A-N7A	-4.37	107.73	113.94
2	A	3001	NDP	C3N-C7N-N7N	4.33	125.36	117.67
2	A	3001	NDP	N3A-C2A-N1A	-4.28	122.11	128.58
2	B	3001	NDP	C5A-C4A-N3A	-4.20	120.93	126.72
2	B	3001	NDP	N9A-C8A-N7A	-4.09	108.14	113.94
2	A	3001	NDP	C5A-C4A-N3A	-4.07	121.11	126.72
2	A	3001	NDP	N9A-C8A-N7A	-4.07	108.17	113.94
2	A	3001	NDP	O2N-PN-O3	4.01	118.11	107.27
2	D	3001	NDP	N9A-C8A-N7A	-4.00	108.26	113.94
2	A	3001	NDP	C5A-N7A-C8A	3.70	109.26	103.45
2	B	3001	NDP	O4B-C1B-N9A	-3.44	101.49	108.09
2	C	3001	NDP	C5A-C4A-N3A	-3.36	122.09	126.72
2	D	3001	NDP	C5A-C4A-N3A	-3.35	122.10	126.72
2	B	3001	NDP	C5A-N7A-C8A	3.29	108.62	103.45
2	D	3001	NDP	N3A-C4A-N9A	3.28	132.75	127.17
2	D	3001	NDP	C4A-N9A-C8A	3.23	109.13	105.74
2	A	3001	NDP	C4A-C5A-N7A	-3.17	106.96	110.58
2	C	3001	NDP	O4B-C1B-N9A	-3.16	102.01	108.09
2	B	3001	NDP	C2A-N3A-C4A	3.10	119.41	111.83
2	D	3001	NDP	O4D-C1D-N1N	2.94	113.70	108.08
2	C	3001	NDP	O3B-C3B-C4B	-2.92	102.69	111.08
2	B	3001	NDP	N3A-C4A-N9A	2.89	132.08	127.17
2	C	3001	NDP	N3A-C4A-N9A	2.88	132.06	127.17
2	C	3001	NDP	C2B-C3B-C4B	2.87	108.17	101.99
2	C	3001	NDP	C2A-N3A-C4A	2.85	118.79	111.83
2	A	3001	NDP	C2A-N3A-C4A	2.82	118.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3001	NDP	O4B-C1B-N9A	-2.81	102.69	108.09
2	D	3001	NDP	C5A-N7A-C8A	2.81	107.86	103.45
2	C	3001	NDP	C5A-N7A-C8A	2.80	107.86	103.45
2	A	3001	NDP	O7N-C7N-C3N	-2.80	115.62	120.90
2	C	3001	NDP	C4A-N9A-C8A	2.78	108.66	105.74
2	D	3001	NDP	O7N-C7N-C3N	-2.61	115.98	120.90
2	B	3001	NDP	O4B-C1B-C2B	-2.59	102.12	106.59
2	D	3001	NDP	O5D-PN-O1N	-2.59	98.67	108.94
2	B	3001	NDP	O2N-PN-O1N	2.53	124.22	112.44
2	C	3001	NDP	C5A-C6A-N6A	-2.50	117.11	123.29
2	D	3001	NDP	O3B-C3B-C4B	-2.49	103.92	111.08
2	D	3001	NDP	C2B-C1B-N9A	2.49	117.86	113.75
2	D	3001	NDP	C2A-N3A-C4A	2.48	117.90	111.83
2	B	3001	NDP	O2B-P2B-O1X	-2.48	100.48	109.33
2	D	3001	NDP	C3N-C7N-N7N	2.42	121.96	117.67
2	A	3001	NDP	C1D-N1N-C2N	-2.39	117.21	121.14
2	D	3001	NDP	P2B-O2B-C2B	-2.38	117.08	123.43
2	C	3001	NDP	C3N-C7N-N7N	2.36	121.86	117.67
2	D	3001	NDP	O5D-C5D-C4D	2.34	116.96	108.99
2	A	3001	NDP	C6A-C5A-C4A	2.33	120.36	117.18
2	D	3001	NDP	C2D-C1D-N1N	-2.32	107.59	113.31
2	A	3001	NDP	O2B-P2B-O1X	-2.30	101.12	109.33
2	D	3001	NDP	C5A-C6A-N6A	-2.20	117.85	123.29
2	D	3001	NDP	N6A-C6A-N1A	2.16	123.18	118.38
2	D	3001	NDP	O2N-PN-O3	2.16	113.10	107.27
2	C	3001	NDP	C3D-C2D-C1D	2.14	105.52	101.46
2	A	3001	NDP	N3A-C4A-N9A	2.13	130.80	127.17
2	B	3001	NDP	O2X-P2B-O2B	2.13	114.15	105.85
2	A	3001	NDP	O5B-PA-O1A	2.12	117.32	108.94
2	B	3001	NDP	P2B-O2B-C2B	-2.10	117.83	123.43
2	D	3001	NDP	C2B-C3B-C4B	2.09	106.50	101.99
2	A	3001	NDP	C5A-C4A-N9A	2.07	108.07	105.81
2	B	3001	NDP	C2B-C3B-C4B	2.06	106.42	101.99
2	D	3001	NDP	C2A-N1A-C6A	2.04	122.09	118.73
2	B	3001	NDP	C4B-O4B-C1B	2.03	113.95	109.47
2	C	3001	NDP	C1D-N1N-C2N	-2.02	117.81	121.14

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	NDP	PN-O3-PA-O5B

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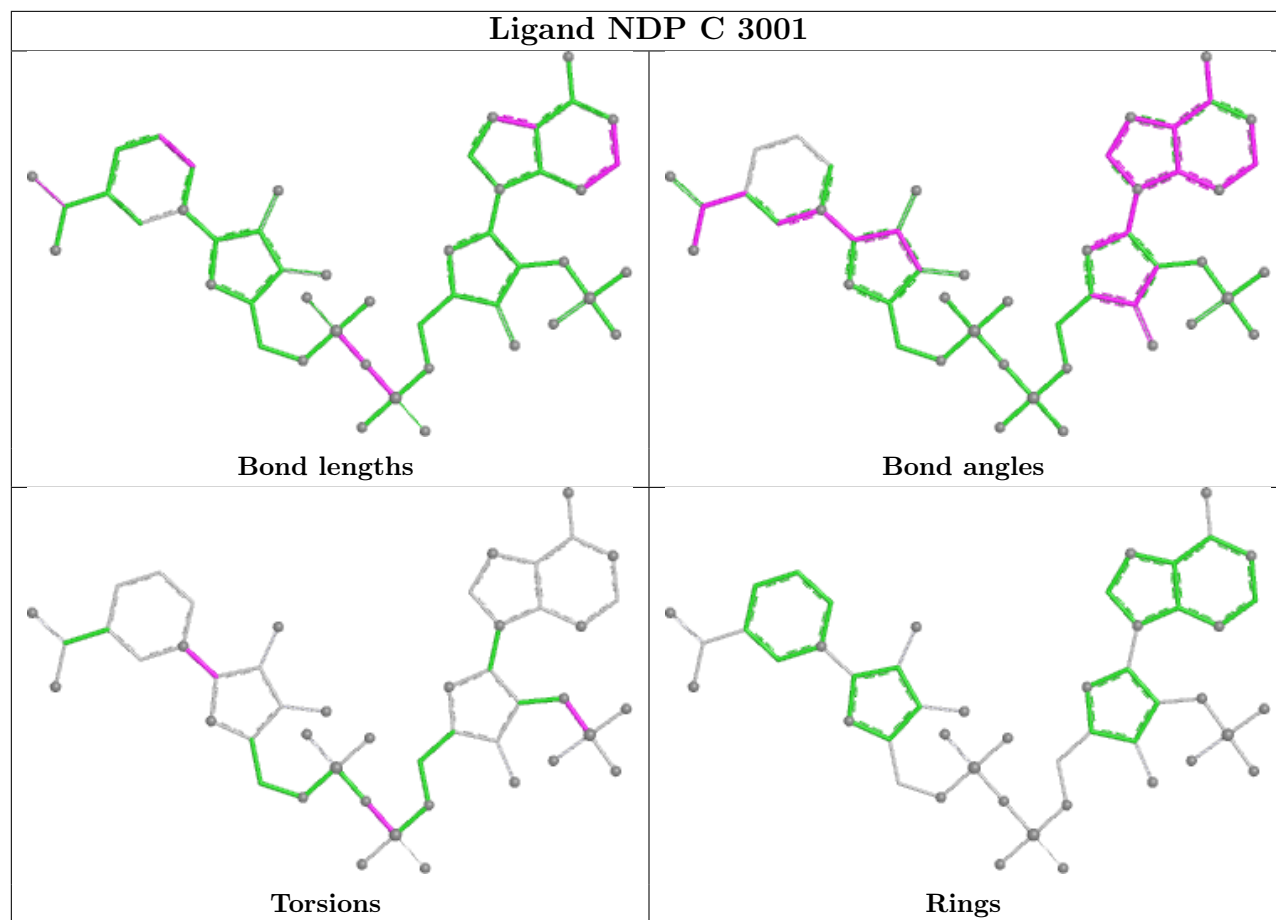
Mol	Chain	Res	Type	Atoms
2	C	3001	NDP	O4D-C1D-N1N-C2N
2	D	3001	NDP	O4D-C1D-N1N-C2N
2	A	3001	NDP	O4D-C1D-N1N-C2N
2	B	3001	NDP	O4D-C1D-N1N-C2N
2	B	3001	NDP	PN-O3-PA-O5B
2	C	3001	NDP	PN-O3-PA-O5B
2	D	3001	NDP	PN-O3-PA-O5B
2	B	3001	NDP	C2B-O2B-P2B-O1X
2	A	3001	NDP	C2B-O2B-P2B-O3X
2	C	3001	NDP	C2B-O2B-P2B-O3X
2	C	3001	NDP	C2B-O2B-P2B-O1X
2	B	3001	NDP	C2B-O2B-P2B-O2X
2	D	3001	NDP	C2B-O2B-P2B-O3X
2	D	3001	NDP	C2B-O2B-P2B-O1X

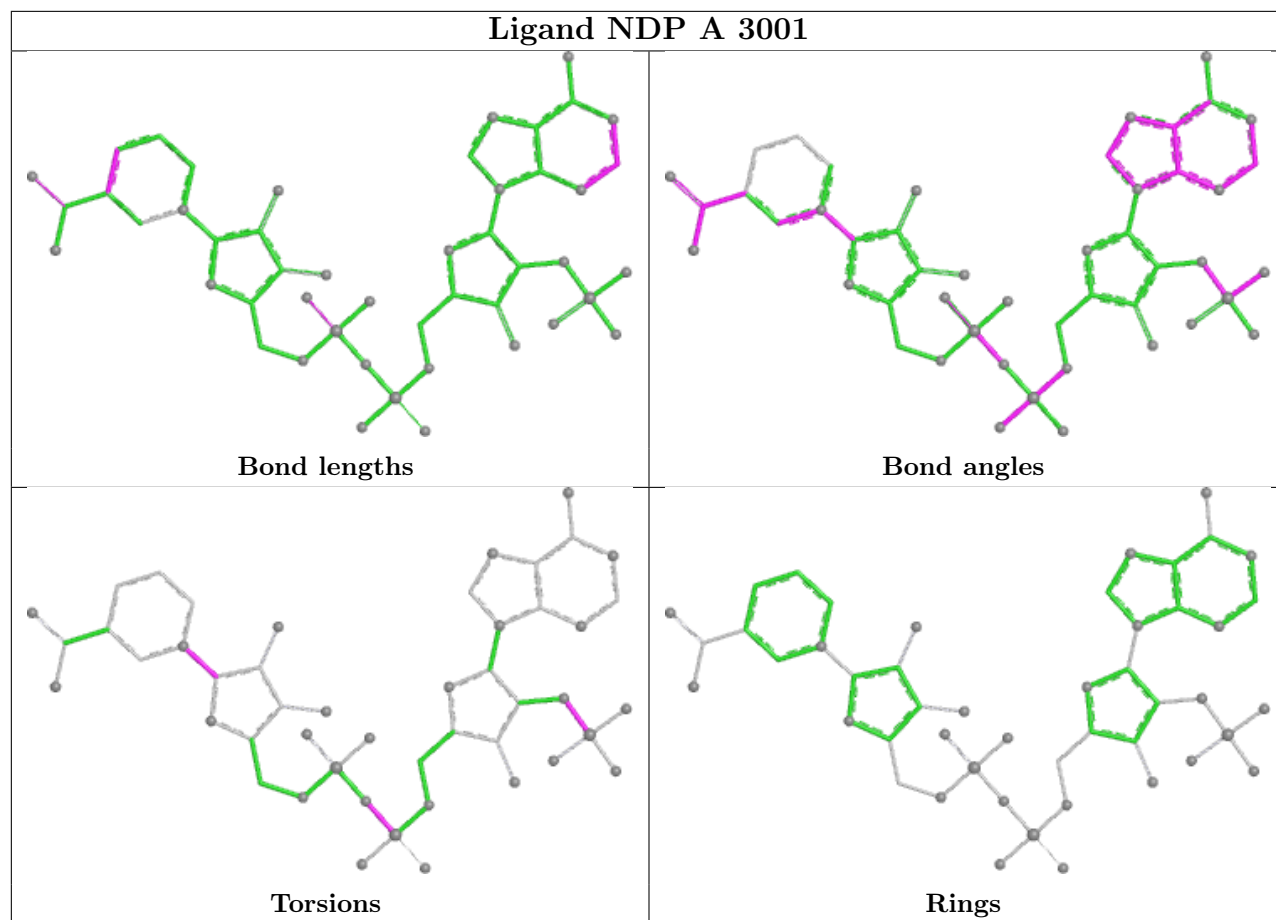
There are no ring outliers.

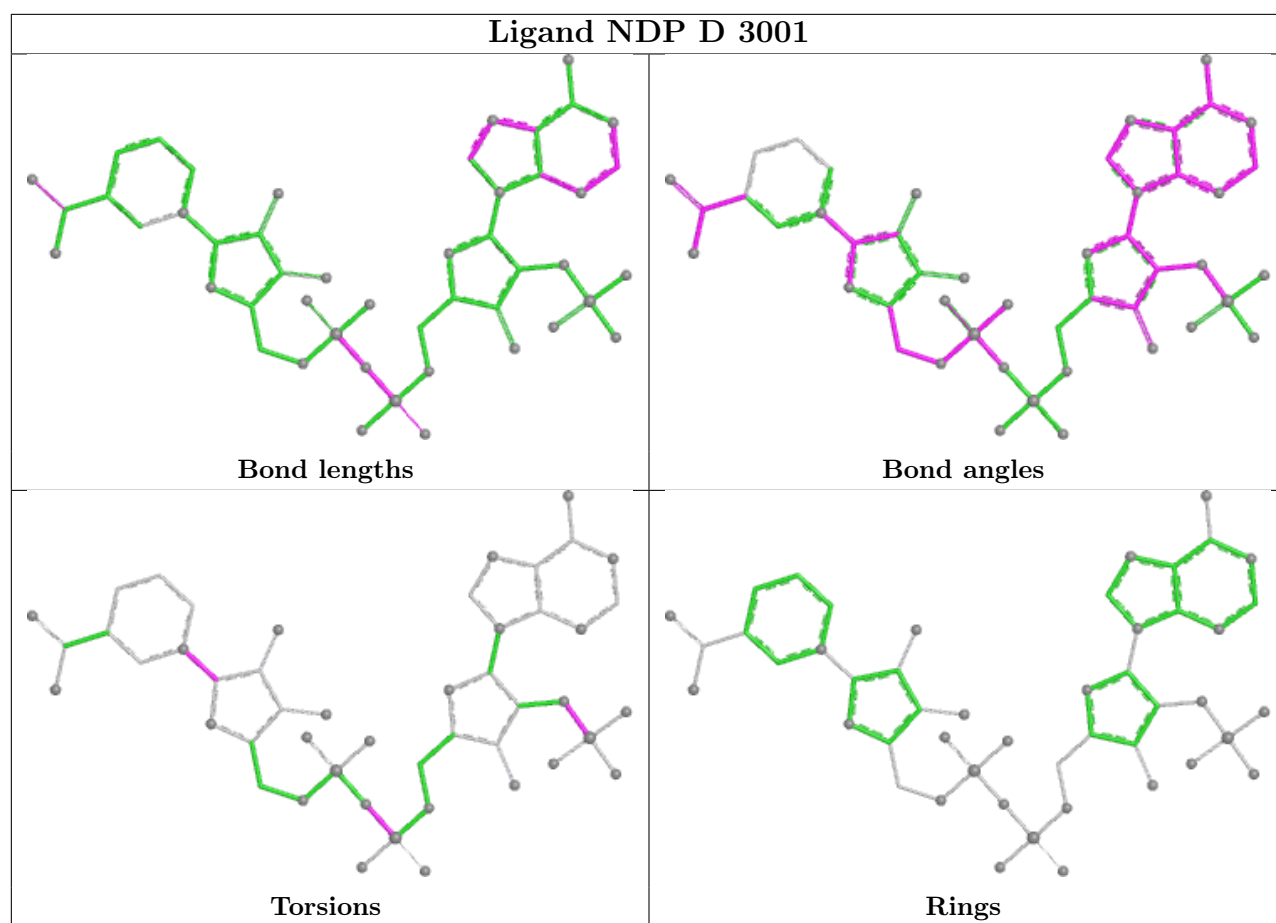
4 monomers are involved in 20 short contacts:

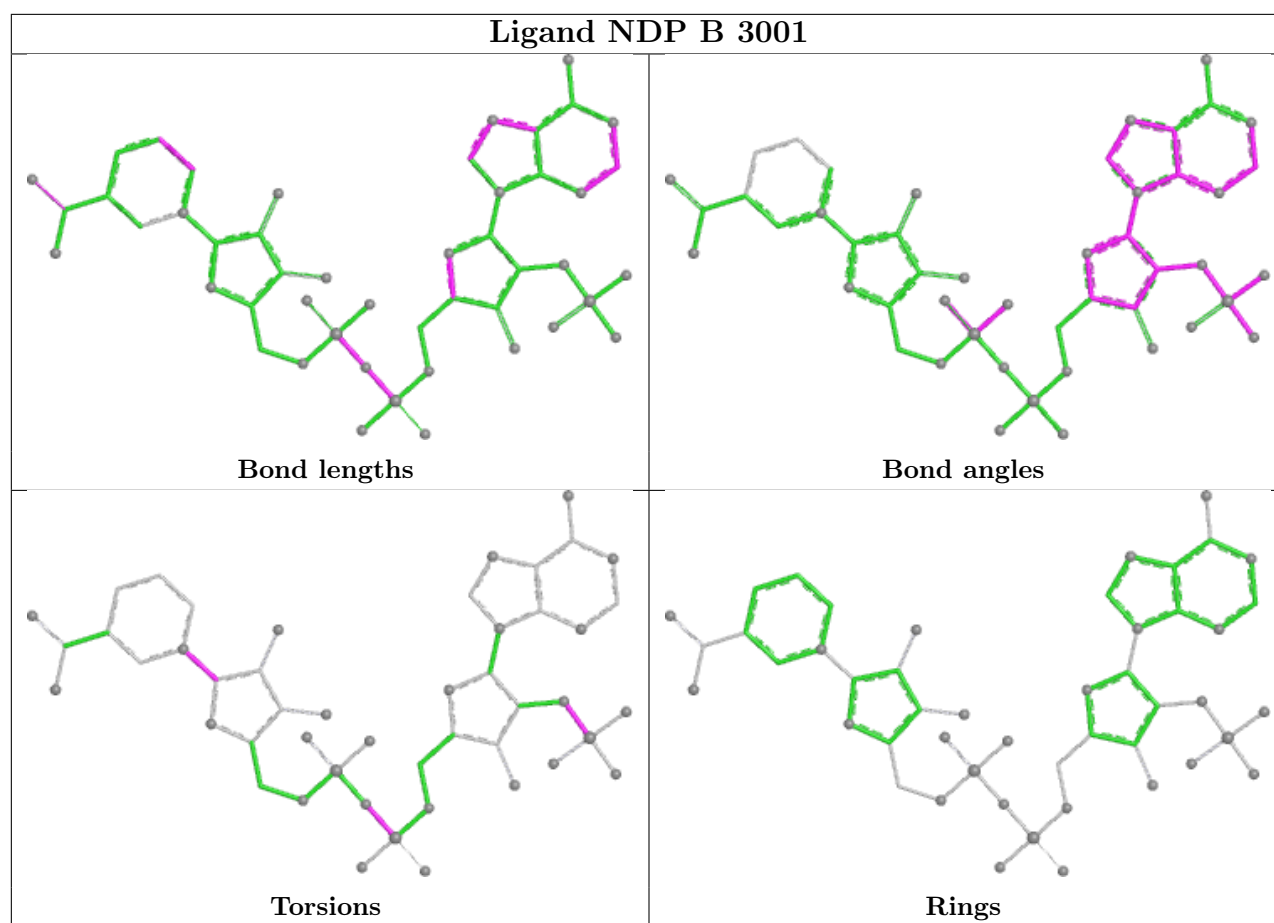
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3001	NDP	4	0
2	A	3001	NDP	6	0
2	D	3001	NDP	6	0
2	B	3001	NDP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	299/307 (97%)	-0.60	0	100	100	18, 30, 47, 59	0
1	B	295/307 (96%)	-0.57	0	100	100	20, 32, 49, 64	0
1	C	298/307 (97%)	-0.67	0	100	100	15, 28, 45, 51	0
1	D	298/307 (97%)	-0.38	1 (0%)	90	88	19, 36, 54, 61	0
All	All	1190/1228 (96%)	-0.56	1 (0%)	92	90	15, 31, 50, 64	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	LYS	2.1

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(Å ²)	Q<0.9
2	NDP	B	3001	48/48	0.96	0.07	10,20,29,35	0

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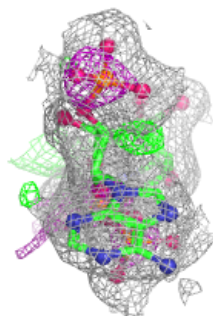
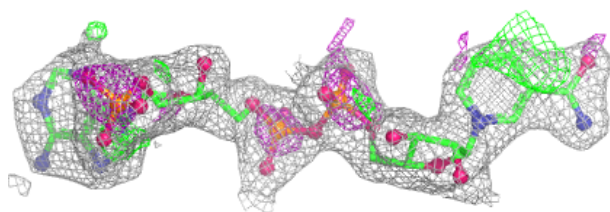
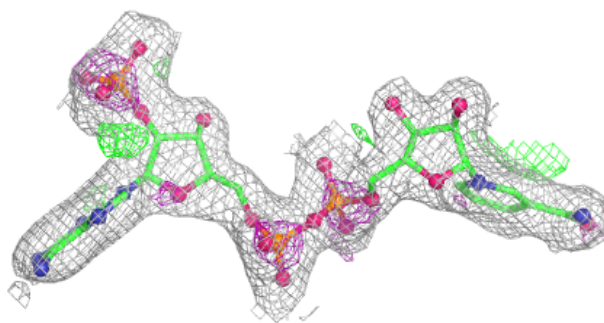
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	A	3001	48/48	0.97	0.06	9,14,23,26	0
2	NDP	D	3001	48/48	0.97	0.05	12,19,23,29	0
2	NDP	C	3001	48/48	0.98	0.04	11,17,24,27	0

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.

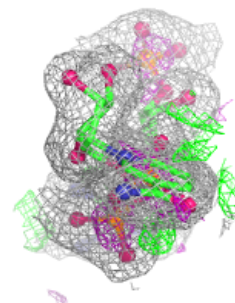
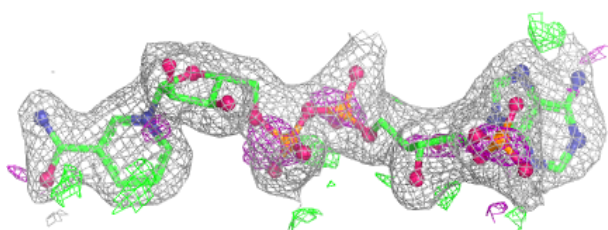
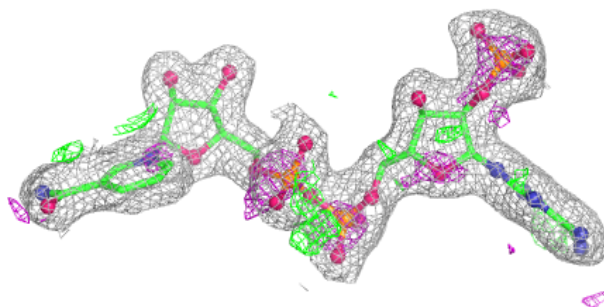
Electron density around NDP B 3001:

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

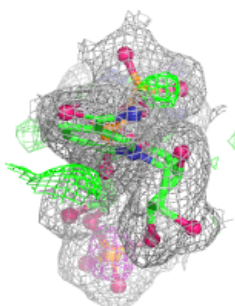
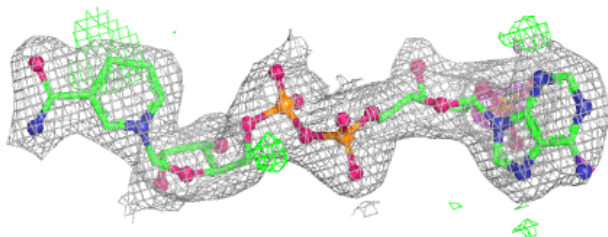
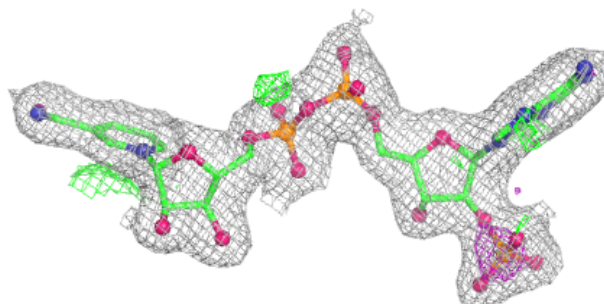


Electron density around NDP A 3001:

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

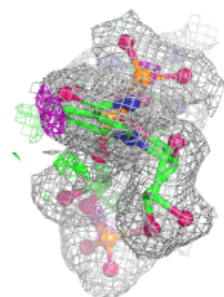
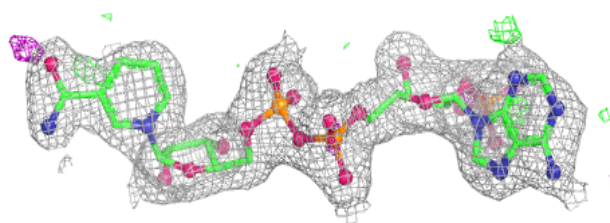
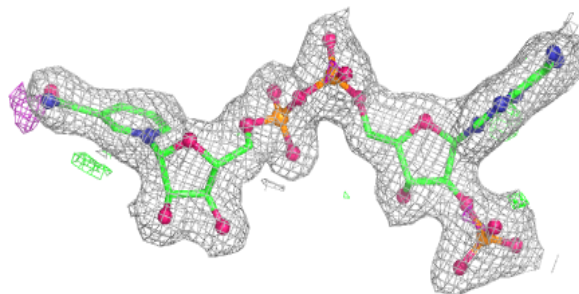
**Electron density around NDP D 3001:**

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



Electron density around NDP C 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.