



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:15 pm BST

PDB ID : 4QUV  
Title : Structure of an integral membrane delta(14)-sterol reductase  
Authors : Li, X.; Blobel, G.  
Deposited on : 2014-07-12  
Resolution : 2.74 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](mailto: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.

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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 : 2.11  
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)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

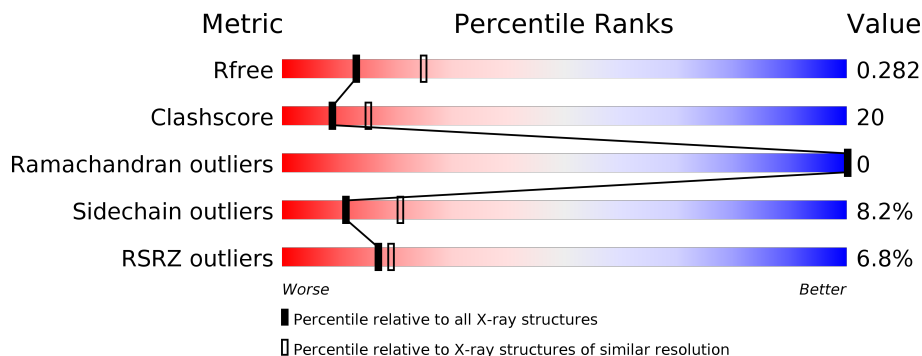
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	427	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">7%      61%      29%      • 8%</p>
1	B	427	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5%      57%      30%      • 9%</p>

## 2 Entry composition [i](#)

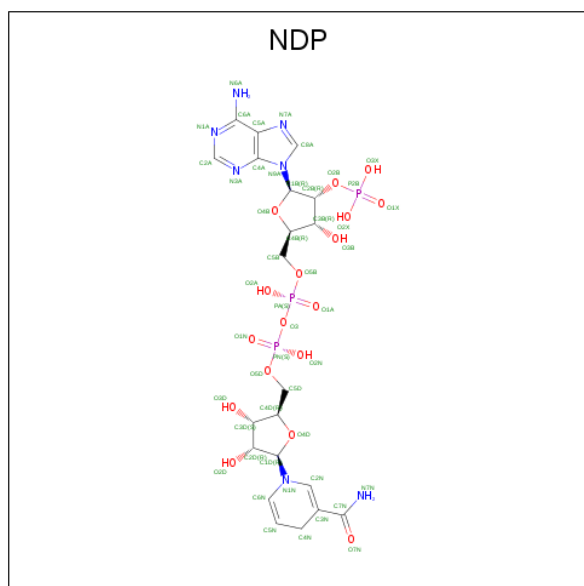
There are 2 unique types of molecules in this entry. The entry contains 6490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Delta(14)-sterol reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	Total	C	N	O	S	0	0	0
			3235	2181	520	516	18			
1	B	389	Total	C	N	O	S	0	0	0
			3193	2149	515	511	18			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.66Å 74.61Å 79.55Å 66.00° 90.37° 86.86°	Depositor
Resolution (Å)	37.26 – 2.74 37.26 – 2.74	Depositor EDS
% Data completeness (in resolution range)	74.5 (37.26-2.74) 74.6 (37.26-2.74)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.72Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.233 , 0.284 0.240 , 0.282	Depositor DCC
$R_{free}$ test set	1527 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.6	Xtrriage
Anisotropy	0.014	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 64.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	0/3360	0.66	1/4590 (0.0%)
1	B	0.51	0/3314	0.72	1/4527 (0.0%)
All	All	0.49	0/6674	0.69	2/9117 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	423	VAL	C-N-CD	5.89	140.77	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3235	0	3203	149	0
1	B	3193	0	3168	116	0
2	A	31	0	11	2	0
2	B	31	0	11	1	0
All	All	6490	0	6393	261	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 20.

All (261) 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:158:GLY:O	1:A:162:PHE:CD2	1.93	1.21
1:A:190:ARG:NH1	1:A:195:ASP:HB2	1.54	1.21
1:A:190:ARG:CZ	1:A:195:ASP:HB2	1.73	1.17
1:A:107:LEU:HD21	1:A:190:ARG:NH2	1.61	1.15
1:A:107:LEU:HD11	1:A:190:ARG:HE	1.13	1.03
1:A:107:LEU:CD2	1:A:190:ARG:NH2	2.25	0.99
1:A:333:LYS:HE2	1:A:336:LYS:HZ3	1.30	0.95
1:B:333:LYS:CG	1:B:334:PRO:HD2	1.97	0.94
1:A:103:ASP:HB3	1:A:105:SER:CB	1.99	0.93
1:A:104:GLY:N	1:A:105:SER:HB3	1.85	0.92
1:A:118:LEU:HD13	1:B:121:LEU:HB3	1.52	0.91
1:A:187:LEU:O	1:A:189:PRO:HD3	1.69	0.91
1:A:158:GLY:O	1:A:162:PHE:HD2	1.41	0.91
1:A:420:TRP:CB	1:A:424:PRO:HB2	1.99	0.90
1:B:188:ASN:OD1	1:B:197:LYS:CD	2.20	0.90
1:A:333:LYS:CE	1:A:336:LYS:HZ3	1.87	0.88
1:A:107:LEU:CD2	1:A:190:ARG:HH21	1.86	0.88
1:A:91:ALA:HB1	1:A:112:ASN:HB3	1.56	0.88
1:A:420:TRP:CD2	1:A:424:PRO:O	2.28	0.86
1:A:57:ALA:HA	1:A:60:ARG:HD3	1.58	0.85
1:A:206:MET:HG3	1:A:275:LEU:HD21	1.59	0.84
1:A:190:ARG:NH1	1:A:195:ASP:CB	2.41	0.83
1:A:333:LYS:HE2	1:A:336:LYS:NZ	1.92	0.82
1:A:107:LEU:HD11	1:A:190:ARG:NE	1.95	0.82
1:B:333:LYS:CD	1:B:334:PRO:HD2	2.10	0.81
1:B:187:LEU:O	1:B:189:PRO:HD3	1.79	0.81
1:A:192:GLY:O	1:A:193:SER:OG	1.99	0.80
1:B:188:ASN:OD1	1:B:197:LYS:HD3	1.79	0.80
1:B:328:ARG:O	1:B:335:ALA:N	2.14	0.80
1:A:355:ALA:HB2	1:A:424:PRO:HB3	1.62	0.79
1:B:99:MET:HG3	1:B:259:LYS:HD3	1.65	0.78
1:B:92:PRO:O	1:B:112:ASN:ND2	2.16	0.78
1:B:188:ASN:OD1	1:B:197:LYS:HD2	1.81	0.78
1:A:420:TRP:HB2	1:A:424:PRO:HB2	1.64	0.77
1:A:107:LEU:HD22	1:A:109:TYR:CZ	2.21	0.76
1:A:103:ASP:HB3	1:A:105:SER:HB3	1.66	0.75
1:A:333:LYS:HG2	1:A:334:PRO:HD2	1.67	0.75
1:A:321:HIS:NE2	1:B:226:THR:HG22	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:OD2	1:A:105:SER:HB2	1.87	0.74
1:B:333:LYS:HD3	1:B:334:PRO:HD2	1.68	0.74
1:A:84:GLN:HE21	1:A:203:ARG:HB3	1.53	0.73
1:A:91:ALA:O	1:A:110:ARG:CZ	2.37	0.72
1:A:420:TRP:CB	1:A:424:PRO:CB	2.67	0.72
1:A:107:LEU:HD22	1:A:109:TYR:CE2	2.25	0.71
1:A:107:LEU:HD21	1:A:190:ARG:CZ	2.20	0.71
1:A:190:ARG:NH2	1:A:195:ASP:HB2	2.04	0.71
1:A:355:ALA:HB2	1:A:424:PRO:CB	2.19	0.71
1:A:337:TYR:HD1	1:A:337:TYR:H	1.39	0.70
1:B:55:ASP:O	1:B:57:ALA:N	2.20	0.70
1:A:355:ALA:HB2	1:A:424:PRO:HG3	1.73	0.70
1:A:333:LYS:CD	1:A:336:LYS:NZ	2.55	0.70
1:A:190:ARG:HH12	1:A:195:ASP:HB2	1.52	0.69
1:B:28:LEU:HD23	1:B:182:PHE:HZ	1.57	0.69
1:A:329:ILE:HG22	1:A:332:GLY:O	1.93	0.69
1:A:423:VAL:HG23	1:A:427:TYR:C	2.12	0.69
1:A:337:TYR:CD2	1:A:345:LEU:HD22	2.28	0.69
1:A:103:ASP:HB3	1:A:105:SER:HB2	1.75	0.68
1:B:333:LYS:HG2	1:B:334:PRO:HD2	1.75	0.68
1:A:99:MET:HG3	1:A:259:LYS:HG2	1.76	0.67
1:B:180:ASP:O	1:B:184:GLY:N	2.28	0.67
1:A:355:ALA:CB	1:A:424:PRO:HB3	2.25	0.67
1:B:99:MET:CE	1:B:259:LYS:HD3	2.24	0.66
1:B:336:LYS:HB2	1:B:349:SER:HB3	1.77	0.66
1:B:333:LYS:CB	1:B:334:PRO:HD2	2.26	0.66
1:A:91:ALA:HB1	1:A:112:ASN:CB	2.25	0.66
1:A:149:VAL:O	1:A:153:THR:HG23	1.96	0.65
1:A:355:ALA:HB2	1:A:424:PRO:CG	2.26	0.65
1:A:333:LYS:CD	1:A:336:LYS:HZ3	2.10	0.65
1:B:187:LEU:HD22	1:B:262:LYS:HG2	1.80	0.65
1:A:420:TRP:HB3	1:A:424:PRO:CB	2.27	0.64
1:A:206:MET:O	1:A:209:TRP:HB3	1.98	0.64
1:B:99:MET:HG3	1:B:259:LYS:CD	2.28	0.64
1:B:99:MET:HE2	1:B:259:LYS:HD3	1.79	0.63
1:A:420:TRP:CG	1:A:424:PRO:O	2.50	0.63
1:A:158:GLY:C	1:A:162:PHE:CD2	2.71	0.63
1:A:423:VAL:HG11	1:A:426:ILE:HB	1.80	0.63
1:B:213:ASN:HB3	1:B:235:VAL:HG22	1.80	0.63
1:A:158:GLY:O	1:A:162:PHE:CE2	2.50	0.62
1:A:216:MET:SD	1:A:284:GLN:HG3	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:MET:HA	1:B:264:GLY:HA3	1.80	0.62
1:B:101:LEU:N	1:B:102:PRO:HD2	2.14	0.61
1:A:107:LEU:HD23	1:A:108:ASP:O	2.00	0.61
1:A:420:TRP:CE3	1:A:424:PRO:O	2.54	0.61
1:B:252:VAL:O	1:B:258:ILE:HG13	2.00	0.61
1:A:91:ALA:O	1:A:110:ARG:NE	2.33	0.61
1:A:104:GLY:H	1:A:105:SER:HB3	1.64	0.60
1:A:158:GLY:C	1:A:162:PHE:HD2	2.04	0.60
1:B:425:LYS:HB3	1:B:426:ILE:HD12	1.84	0.60
1:B:58:ALA:O	1:B:62:PHE:N	2.32	0.60
1:A:121:LEU:HB3	1:B:118:LEU:HD13	1.84	0.59
1:A:107:LEU:HD22	1:A:190:ARG:HH21	1.66	0.58
1:B:395:ARG:HG3	1:B:398:ARG:HH22	1.67	0.58
1:B:112:ASN:OD1	1:B:115:PHE:HB3	2.03	0.58
1:B:206:MET:HG3	1:B:275:LEU:HD21	1.85	0.58
1:B:149:VAL:O	1:B:153:THR:HG23	2.04	0.58
1:A:139:TYR:HD2	1:A:216:MET:HG2	1.70	0.57
1:A:420:TRP:CG	1:A:424:PRO:HB2	2.40	0.57
1:B:161:TYR:HE1	1:B:180:ASP:HB2	1.68	0.57
1:A:161:TYR:HE1	1:A:180:ASP:HB2	1.68	0.57
1:A:337:TYR:N	1:A:337:TYR:CD1	2.72	0.57
1:A:93:GLY:N	1:A:112:ASN:OD1	2.28	0.57
1:A:99:MET:CE	1:A:259:LYS:HD3	2.35	0.56
1:B:216:MET:SD	1:B:284:GLN:HG3	2.45	0.56
1:A:107:LEU:HD22	1:A:190:ARG:NH2	2.17	0.56
1:A:423:VAL:CG2	1:A:427:TYR:H	2.19	0.56
1:B:97:GLN:HB3	1:B:106:ARG:HG2	1.86	0.56
1:A:134:ASP:O	1:A:137:VAL:HG23	2.06	0.56
1:B:147:THR:O	1:B:151:ILE:HG23	2.06	0.56
1:B:124:VAL:HG11	1:B:211:LEU:HD22	1.88	0.56
1:A:185:THR:O	1:A:186:ALA:HB3	2.06	0.56
1:A:420:TRP:HB2	1:A:424:PRO:CB	2.31	0.55
1:A:183:MET:O	1:A:262:LYS:O	2.24	0.55
1:B:357:HIS:N	1:B:421:ARG:O	2.39	0.55
1:A:100:LYS:HB3	1:A:105:SER:HG	1.72	0.55
1:A:333:LYS:HD3	1:A:336:LYS:NZ	2.22	0.55
1:B:101:LEU:N	1:B:102:PRO:CD	2.68	0.55
1:B:378:SER:O	1:B:381:PRO:HD2	2.07	0.55
1:B:102:PRO:O	1:B:103:ASP:HB3	2.07	0.54
1:A:190:ARG:CZ	1:A:195:ASP:CB	2.67	0.54
1:B:43:VAL:HA	1:B:48:GLY:HA2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:MET:HE2	1:B:259:LYS:CD	2.38	0.54
1:A:333:LYS:CE	1:A:336:LYS:NZ	2.58	0.54
1:A:240:PHE:HA	1:A:243:ILE:HD12	1.89	0.53
1:B:146:LEU:HD13	1:B:277:PHE:CD2	2.43	0.53
1:A:329:ILE:CG2	1:A:332:GLY:O	2.56	0.53
1:B:187:LEU:O	1:B:189:PRO:CD	2.56	0.53
1:B:338:ILE:HD11	1:B:417:LYS:HG3	1.89	0.53
1:B:177:PRO:HB2	1:B:179:TYR:HD1	1.74	0.52
1:A:139:TYR:CE2	1:A:287:VAL:HG11	2.44	0.52
1:A:228:THR:HG21	1:A:290:THR:HA	1.90	0.52
1:B:134:ASP:O	1:B:137:VAL:HG23	2.09	0.52
1:B:228:THR:HG21	1:B:290:THR:HA	1.92	0.52
1:B:99:MET:HG3	1:B:259:LYS:HG2	1.92	0.52
1:A:48:GLY:O	1:A:378:SER:OG	2.22	0.52
1:A:407:TYR:HB2	1:A:411:TRP:HB2	1.92	0.52
1:A:107:LEU:CD2	1:A:108:ASP:O	2.59	0.51
1:A:252:VAL:O	1:A:255:THR:HG22	2.11	0.51
1:B:84:GLN:HB3	1:B:203:ARG:HB3	1.93	0.51
1:A:325:ASP:HB3	1:A:328:ARG:HG3	1.93	0.51
1:A:28:LEU:HD23	1:A:182:PHE:HZ	1.76	0.51
1:A:413:GLN:HA	1:A:416:LYS:HD2	1.92	0.51
1:A:423:VAL:HG21	1:A:427:TYR:N	2.26	0.50
1:A:370:TRP:O	1:A:373:PRO:HD2	2.11	0.50
1:B:40:TRP:CE3	1:B:142:LEU:HD22	2.47	0.50
1:A:285:TYR:CE2	1:A:378:SER:HB3	2.46	0.50
1:A:179:TYR:O	1:A:182:PHE:N	2.38	0.50
1:A:88:GLN:HA	1:A:203:ARG:HH12	1.77	0.50
1:B:347:LEU:HD22	1:B:349:SER:H	1.76	0.50
1:B:101:LEU:HD22	1:B:106:ARG:HH22	1.76	0.50
1:A:321:HIS:CE1	1:B:226:THR:HG22	2.48	0.49
1:A:84:GLN:HB3	1:A:203:ARG:HB3	1.93	0.49
1:A:275:LEU:HD12	1:A:279:TYR:CZ	2.47	0.49
1:B:36:VAL:HG12	1:B:146:LEU:HD21	1.94	0.49
1:A:254:THR:O	1:A:259:LYS:HE2	2.12	0.49
1:A:318:GLN:OE1	1:A:350:GLY:HA3	2.12	0.49
1:B:309:TYR:HA	1:B:366:ILE:HD11	1.94	0.49
1:B:99:MET:HG3	1:B:259:LYS:CG	2.42	0.49
1:B:368:LEU:HD13	1:B:385:ILE:HG13	1.94	0.49
1:B:91:ALA:HB1	1:B:112:ASN:HB3	1.94	0.48
1:A:100:LYS:HB3	1:A:105:SER:OG	2.12	0.48
1:A:423:VAL:HG21	1:A:427:TYR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:HG2	1:A:253:LEU:O	2.14	0.48
2:A:501:NDP:H8A	2:A:501:NDP:H3B	1.96	0.48
1:B:40:TRP:CZ3	1:B:142:LEU:HD22	2.49	0.48
1:A:103:ASP:CB	1:A:105:SER:HB2	2.42	0.48
1:B:161:TYR:CE1	1:B:180:ASP:HB2	2.48	0.48
1:B:385:ILE:HA	1:B:385:ILE:HD13	1.59	0.47
1:B:107:LEU:HD22	1:B:190:ARG:NH2	2.29	0.47
1:B:298:ILE:O	1:B:302:VAL:HG22	2.15	0.47
1:A:213:ASN:HB3	1:A:235:VAL:HG23	1.96	0.47
1:B:275:LEU:O	1:B:279:TYR:HB2	2.14	0.47
1:B:400:ASP:OD1	1:B:415:ARG:NH2	2.48	0.47
1:B:356:ARG:NH1	1:B:415:ARG:HG2	2.30	0.47
1:B:101:LEU:HB2	1:B:102:PRO:HD3	1.97	0.47
1:A:99:MET:HG3	1:A:259:LYS:CG	2.43	0.47
1:A:322:PHE:CG	1:A:347:LEU:HD13	2.50	0.47
1:B:87:LEU:O	1:B:91:ALA:N	2.47	0.46
1:A:224:HIS:CG	1:A:290:THR:HG21	2.50	0.46
1:A:413:GLN:O	1:A:416:LYS:HB2	2.15	0.46
1:B:190:ARG:HG2	1:B:195:ASP:HA	1.98	0.46
1:B:206:MET:O	1:B:209:TRP:HB3	2.15	0.46
1:A:347:LEU:N	2:A:501:NDP:N1A	2.60	0.46
1:B:121:LEU:HD13	1:B:121:LEU:HA	1.69	0.46
1:B:333:LYS:HG2	1:B:334:PRO:CD	2.44	0.46
1:B:354:ILE:HG22	1:B:424:PRO:HG3	1.98	0.46
1:A:231:MET:O	1:A:235:VAL:HG12	2.16	0.46
1:A:99:MET:SD	1:A:259:LYS:HD3	2.55	0.46
1:B:100:LYS:HD2	1:B:105:SER:O	2.14	0.46
1:B:138:LEU:HB3	1:B:212:MET:HG2	1.96	0.46
1:B:99:MET:HB3	1:B:100:LYS:H	1.62	0.45
1:B:115:PHE:CD1	1:B:115:PHE:C	2.88	0.45
1:B:313:ARG:O	1:B:317:ILE:HG23	2.17	0.45
1:B:99:MET:CG	1:B:259:LYS:HD3	2.40	0.45
1:B:388:PHE:CE2	1:B:392:LEU:HD11	2.51	0.45
1:A:393:LEU:HA	1:A:393:LEU:HD23	1.82	0.45
1:A:412:LEU:O	1:A:416:LYS:HG3	2.15	0.45
1:B:302:VAL:O	1:B:306:LEU:HG	2.17	0.45
1:B:333:LYS:CB	1:B:334:PRO:CD	2.93	0.45
1:A:107:LEU:HD13	1:A:188:ASN:ND2	2.32	0.45
1:A:102:PRO:O	1:A:103:ASP:CB	2.65	0.45
1:B:70:THR:HG23	1:B:73:ALA:H	1.82	0.45
1:B:98:GLY:HA3	1:B:109:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:HIS:CE1	1:B:313:ARG:NH1	2.86	0.44
1:B:209:TRP:HH2	1:B:370:TRP:CH2	2.35	0.44
1:A:87:LEU:HD21	1:A:119:PHE:CD2	2.52	0.44
1:A:216:MET:HE3	1:A:283:ALA:HB3	2.00	0.44
1:A:115:PHE:CD1	1:A:115:PHE:C	2.91	0.43
1:A:191:ILE:O	1:A:194:LEU:HB3	2.18	0.43
1:A:45:TYR:N	1:A:45:TYR:CD1	2.85	0.43
1:A:102:PRO:O	1:A:103:ASP:HB3	2.16	0.43
1:B:347:LEU:N	2:B:501:NDP:N1A	2.55	0.43
1:A:230:PRO:HG3	1:A:293:LEU:CD2	2.48	0.43
1:A:339:LYS:HE3	1:A:339:LYS:HB2	1.72	0.43
1:B:206:MET:HG3	1:B:275:LEU:CD2	2.48	0.43
1:B:323:ARG:NH2	1:B:345:LEU:O	2.47	0.43
1:A:188:ASN:OD1	1:A:188:ASN:N	2.50	0.43
1:B:53:THR:HB	1:B:55:ASP:H	1.84	0.43
1:A:107:LEU:CD1	1:A:190:ARG:HH21	2.32	0.43
1:A:203:ARG:HB2	1:A:204:PRO:HD3	2.01	0.43
1:B:243:ILE:HD12	1:B:243:ILE:HG23	1.76	0.43
1:A:99:MET:HG3	1:A:259:LYS:HD3	2.00	0.43
1:A:423:VAL:CG2	1:A:427:TYR:N	2.82	0.42
1:B:59:TRP:CE3	1:B:59:TRP:HA	2.54	0.42
1:B:141:GLN:O	1:B:145:LEU:HG	2.20	0.42
1:A:190:ARG:HG2	1:A:195:ASP:HA	2.01	0.42
1:A:196:LEU:CB	1:A:263:PHE:HE2	2.33	0.42
1:B:212:MET:HE3	1:B:280:THR:HG21	2.00	0.42
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.45	0.42
1:A:124:VAL:HG11	1:A:211:LEU:HD22	2.01	0.42
1:A:99:MET:HG3	1:A:259:LYS:CD	2.50	0.42
1:B:91:ALA:CB	1:B:112:ASN:HB3	2.49	0.42
1:A:253:LEU:HA	1:A:253:LEU:HD23	1.92	0.42
1:B:339:LYS:HE3	1:B:339:LYS:HB2	1.76	0.41
1:A:216:MET:HB2	1:A:216:MET:HE2	1.80	0.41
1:A:91:ALA:O	1:A:110:ARG:NH2	2.53	0.41
1:A:347:LEU:HD23	1:A:352:TRP:CD1	2.55	0.41
1:B:242:LEU:O	1:B:245:TYR:HB3	2.20	0.41
1:B:197:LYS:NZ	1:B:261:GLU:O	2.35	0.41
1:B:333:LYS:CG	1:B:334:PRO:CD	2.86	0.41
1:A:213:ASN:ND2	1:A:238:GLN:OE1	2.53	0.41
1:B:95:THR:HA	1:B:110:ARG:HA	2.02	0.41
1:B:203:ARG:HB2	1:B:204:PRO:HD3	2.02	0.41
1:B:87:LEU:O	1:B:91:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.84	0.41
1:B:256:TRP:CE2	1:B:398:ARG:HD2	2.55	0.41
1:B:423:VAL:HB	1:B:427:TYR:H	1.85	0.41
1:B:380:ILE:HB	1:B:381:PRO:HD3	2.01	0.41
1:A:357:HIS:N	1:A:421:ARG:O	2.54	0.41
1:B:134:ASP:OD1	1:B:134:ASP:N	2.54	0.41
1:B:151:ILE:O	1:B:155:VAL:HG12	2.20	0.41
1:B:204:PRO:O	1:B:208:PHE:HB2	2.20	0.41
1:B:45:TYR:CD2	1:B:65:HIS:CD2	3.08	0.41
1:A:317:ILE:HG22	1:A:321:HIS:CD2	2.56	0.41
1:A:145:LEU:HD13	1:A:208:PHE:HZ	1.86	0.41
1:A:252:VAL:O	1:A:258:ILE:HG13	2.20	0.41
1:B:423:VAL:H	1:B:427:TYR:C	2.25	0.41
1:A:329:ILE:HG13	1:A:329:ILE:H	1.58	0.41
1:B:234:VAL:HG23	1:B:373:PRO:HG2	2.02	0.41
1:A:344:SER:HB2	1:A:407:TYR:HE1	1.86	0.40
1:A:275:LEU:HD12	1:A:279:TYR:CE2	2.56	0.40
1:A:321:HIS:NE2	1:B:226:THR:CG2	2.79	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	389/427 (91%)	353 (91%)	36 (9%)	0	100	100
1	B	385/427 (90%)	349 (91%)	36 (9%)	0	100	100
All	All	774/854 (91%)	702 (91%)	72 (9%)	0	100	100

There are no Ramachandran outliers to report.

### 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	331/358 (92%)	305 (92%)	26 (8%)	12	22
1	B	327/358 (91%)	299 (91%)	28 (9%)	10	19
All	All	658/716 (92%)	604 (92%)	54 (8%)	11	21

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	CYS
1	A	92	PRO
1	A	100	LYS
1	A	110	ARG
1	A	112	ASN
1	A	120	THR
1	A	121	LEU
1	A	127	LEU
1	A	129	THR
1	A	134	ASP
1	A	146	LEU
1	A	156	PHE
1	A	163	TRP
1	A	179	TYR
1	A	187	LEU
1	A	196	LEU
1	A	219	LYS
1	A	227	VAL
1	A	229	VAL
1	A	263	PHE
1	A	267	LEU
1	A	281	LEU
1	A	282	GLN
1	A	293	LEU
1	A	295	VAL
1	A	337	TYR
1	B	42	CYS

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Mol	Chain	Res	Type
1	B	120	THR
1	B	121	LEU
1	B	127	LEU
1	B	134	ASP
1	B	151	ILE
1	B	179	TYR
1	B	183	MET
1	B	187	LEU
1	B	201	GLU
1	B	206	MET
1	B	216	MET
1	B	229	VAL
1	B	250	GLU
1	B	263	PHE
1	B	267	LEU
1	B	280	THR
1	B	281	LEU
1	B	288	HIS
1	B	306	LEU
1	B	317	ILE
1	B	329	ILE
1	B	333	LYS
1	B	337	TYR
1	B	347	LEU
1	B	385	ILE
1	B	416	LYS
1	B	421	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NDP	A	501	-	27,33,52	1.17	2 (7%)	35,52,80	1.34	5 (14%)
2	NDP	B	501	-	27,33,52	1.16	3 (11%)	35,52,80	1.29	4 (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	501	-	-	7/17/37/77	0/3/3/5
2	NDP	B	501	-	-	10/17/37/77	0/3/3/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NDP	C5A-C4A	3.13	1.49	1.40
2	B	501	NDP	C5A-C4A	2.87	1.48	1.40
2	A	501	NDP	C2A-N3A	2.41	1.36	1.32
2	B	501	NDP	C2A-N3A	2.36	1.35	1.32
2	B	501	NDP	P2B-O2B	2.14	1.63	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NDP	N3A-C2A-N1A	-3.52	123.17	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NDP	PA-O3-PN	-3.38	121.23	132.83
2	A	501	NDP	PA-O3-PN	-3.02	122.47	132.83
2	A	501	NDP	N3A-C2A-N1A	-2.73	124.41	128.68
2	A	501	NDP	O2B-C2B-C3B	-2.63	102.15	111.68
2	B	501	NDP	O2N-PN-O1N	2.60	120.85	110.68
2	A	501	NDP	O2N-PN-O1N	2.60	120.84	110.68
2	B	501	NDP	O2B-C2B-C3B	-2.18	103.79	111.68
2	A	501	NDP	O4B-C1B-C2B	-2.12	102.91	106.59

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	C3B-C4B-C5B-O5B
2	B	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	C3B-C4B-C5B-O5B
2	A	501	NDP	C3B-C2B-O2B-P2B
2	B	501	NDP	C3B-C2B-O2B-P2B
2	A	501	NDP	PN-O3-PA-O5B
2	B	501	NDP	PA-O3-PN-O1N
2	B	501	NDP	PA-O3-PN-O2N
2	A	501	NDP	C5B-O5B-PA-O1A
2	B	501	NDP	C5B-O5B-PA-O1A
2	A	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	C1B-C2B-O2B-P2B
2	A	501	NDP	C1B-C2B-O2B-P2B
2	B	501	NDP	PA-O3-PN-O5D
2	B	501	NDP	C2B-O2B-P2B-O3X

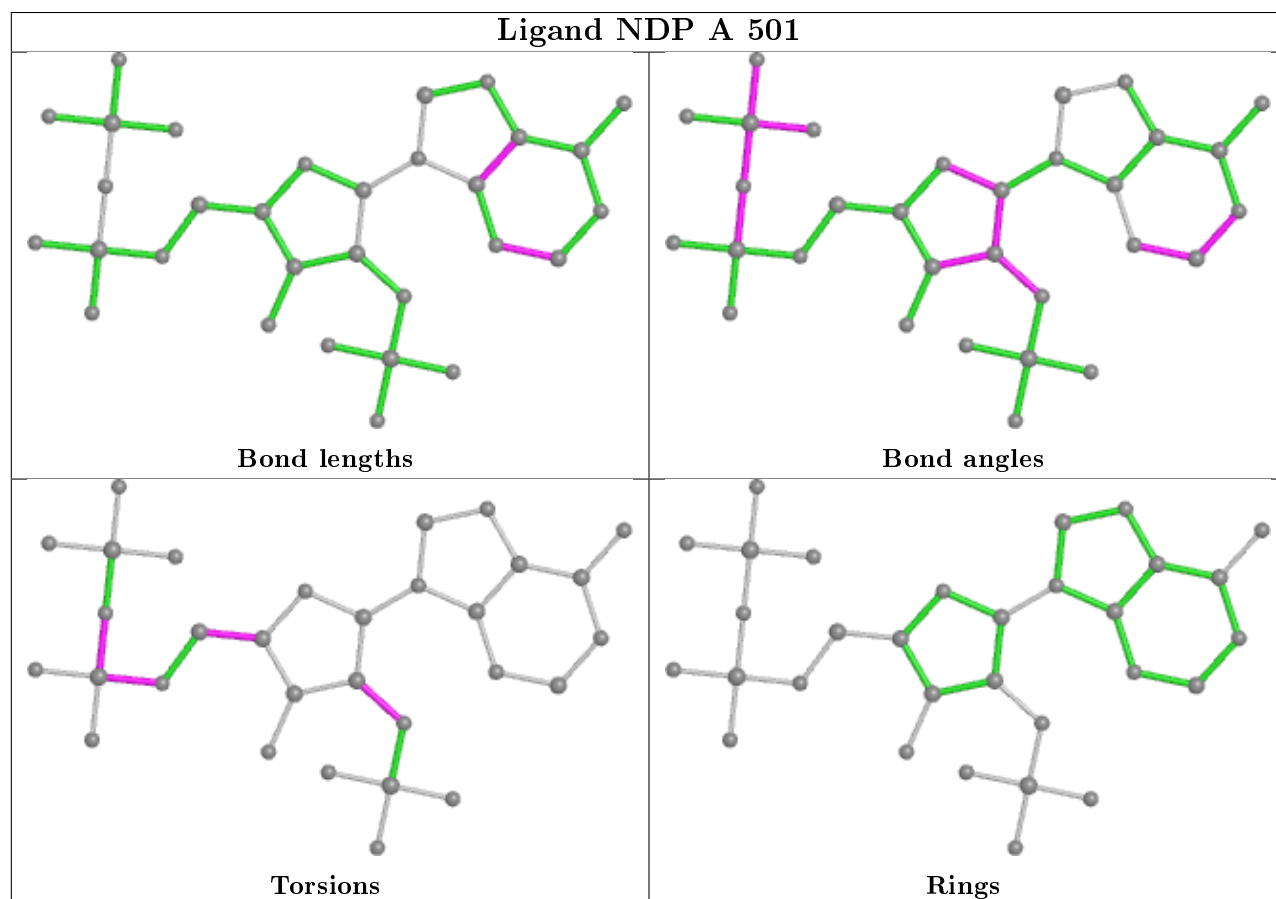
There are no ring outliers.

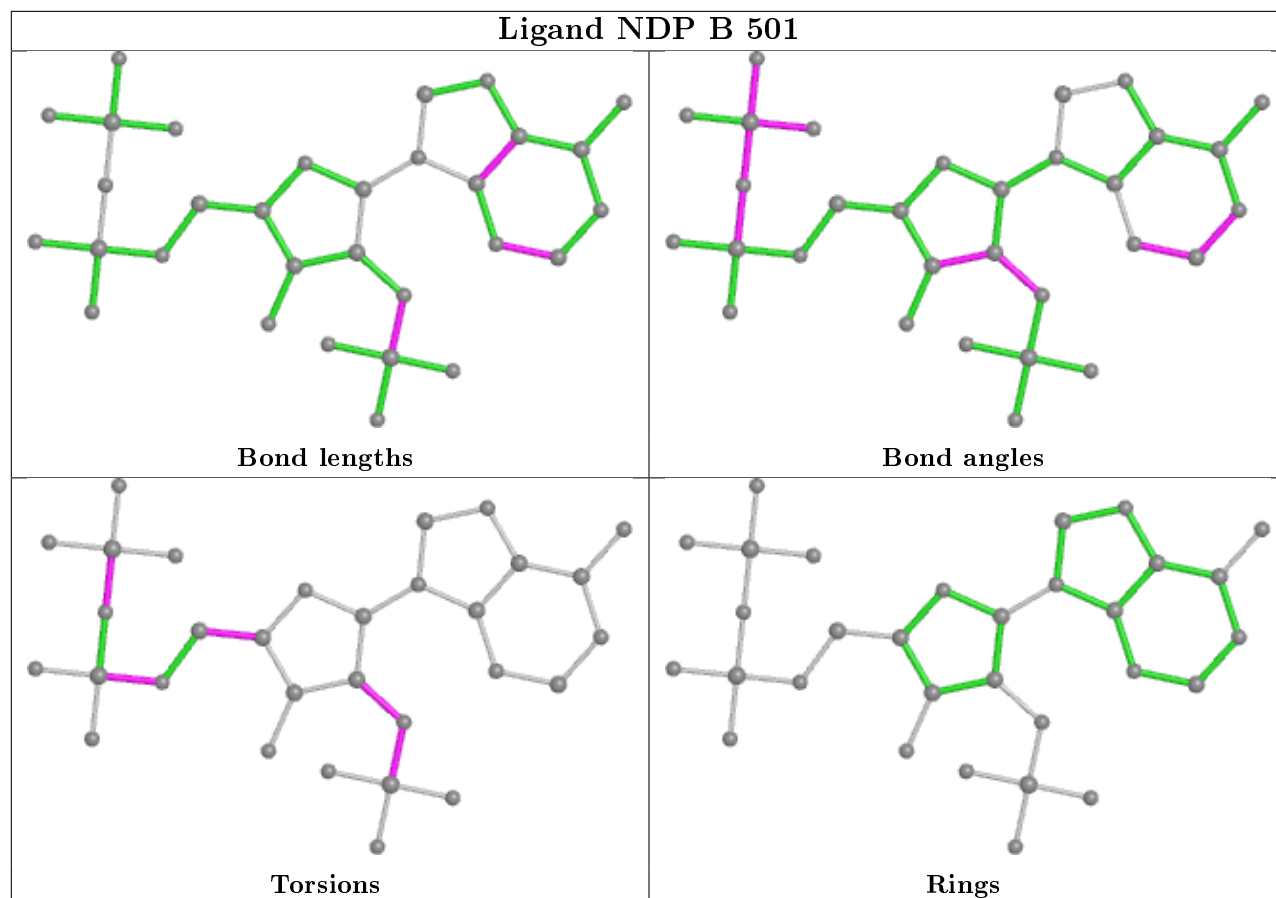
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	2	0
2	B	501	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	393/427 (92%)	0.38	31 (7%) 12 14	47, 86, 148, 227	0
1	B	389/427 (91%)	0.20	22 (5%) 23 26	42, 82, 139, 239	0
All	All	782/854 (91%)	0.29	53 (6%) 17 19	42, 84, 145, 239	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	PHE	10.5
1	A	186	ALA	7.0
1	A	177	PRO	7.0
1	B	102	PRO	6.2
1	B	105	SER	5.5
1	A	185	THR	4.8
1	A	328	ARG	4.6
1	A	162	PHE	4.6
1	B	52	PHE	4.2
1	B	332	GLY	4.2
1	A	327	ASN	4.1
1	A	23	PHE	3.9
1	A	187	LEU	3.9
1	B	193	SER	3.8
1	B	327	ASN	3.8
1	A	424	PRO	3.7
1	B	101	LEU	3.4
1	A	426	ILE	3.4
1	A	59	TRP	3.4
1	A	54	SER	3.3
1	A	102	PRO	3.3
1	A	324	ARG	3.1
1	B	71	TRP	3.1
1	A	26	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	333	LYS	3.0
1	B	328	ARG	2.9
1	A	160	LEU	2.9
1	B	103	ASP	2.8
1	A	99	MET	2.8
1	B	90	TRP	2.8
1	A	262	LYS	2.7
1	A	180	ASP	2.5
1	A	179	TYR	2.5
1	A	423	VAL	2.4
1	B	334	PRO	2.4
1	B	341	LYS	2.4
1	A	333	LYS	2.3
1	B	182	PHE	2.3
1	B	185	THR	2.3
1	A	61	ARG	2.3
1	A	263	PHE	2.3
1	B	330	VAL	2.3
1	A	101	LEU	2.2
1	B	261	GLU	2.2
1	A	329	ILE	2.2
1	B	263	PHE	2.2
1	A	325	ASP	2.1
1	B	260	HIS	2.1
1	B	94	PRO	2.1
1	A	66	VAL	2.1
1	B	92	PRO	2.1
1	A	72	HIS	2.0
1	A	90	TRP	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](#)

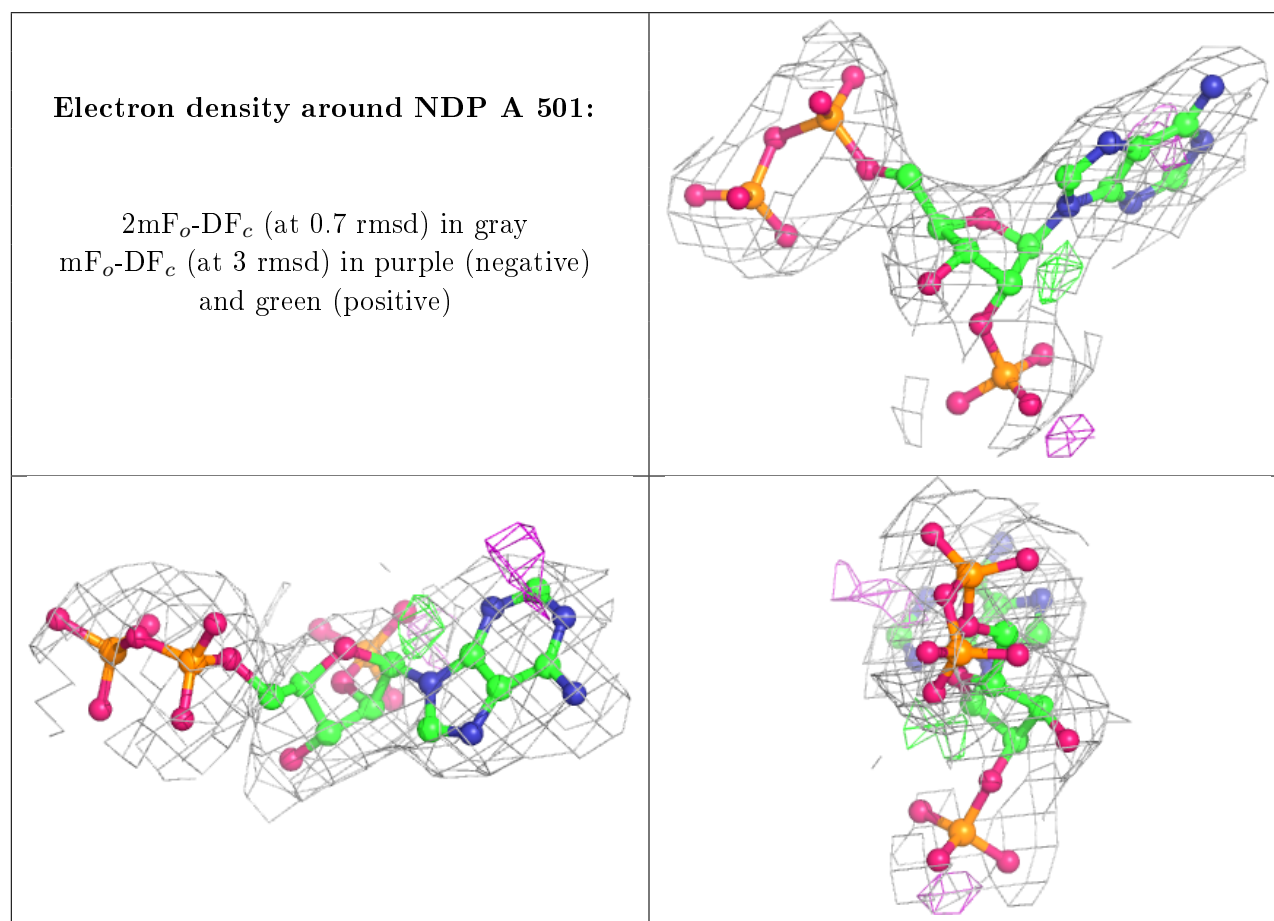
There are no carbohydrates in this entry.

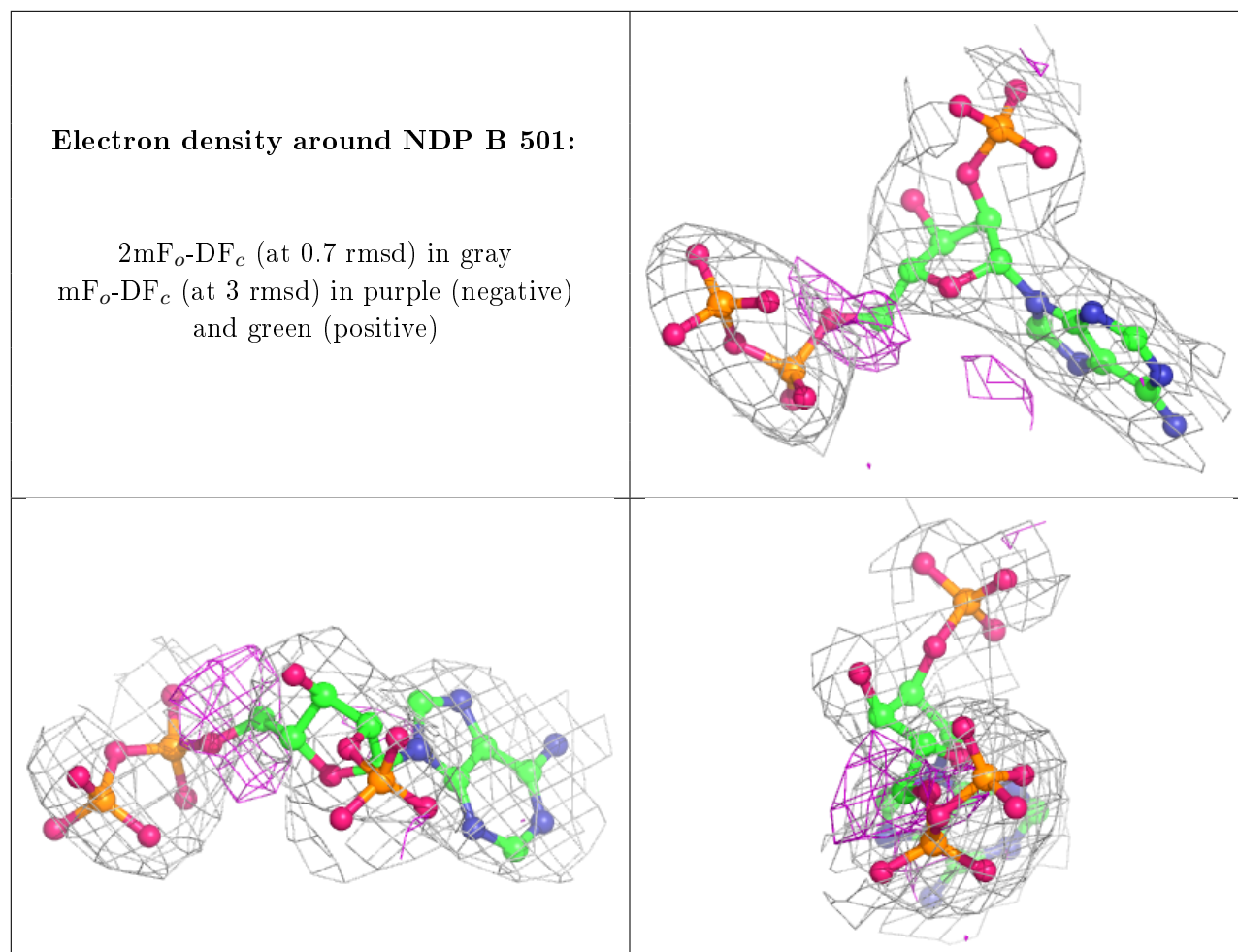
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDP	A	501	31/48	0.89	0.17	41,77,119,301	0
2	NDP	B	501	31/48	0.92	0.15	46,89,114,364	0

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.