



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:38 am BST

PDB ID : 3OJF  
Title : Crystal Structure of the Bacillus cereus Enoyl-Acyl Carrier Protein Reductase with NADP<sup>+</sup> and indole naphthyridinone (Complex form)  
Authors : Kim, S.J.; Ha, B.H.; Kim, K.H.; Hong, S.K.; Suh, S.W.; Kim, E.E.  
Deposited on : 2010-08-22  
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](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

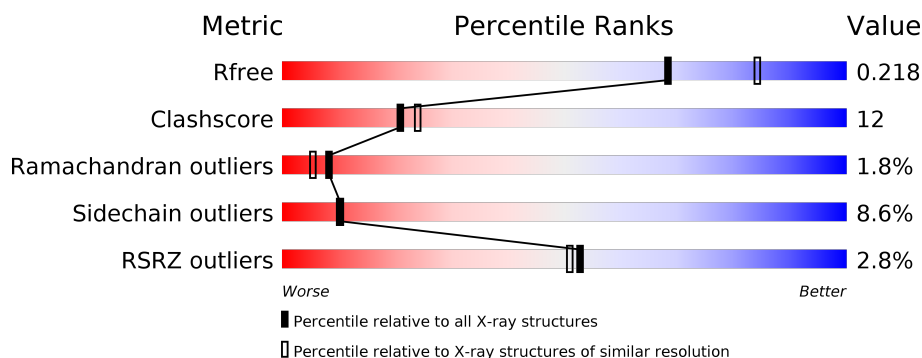
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	257	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	257	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	257	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>7%</div> </div> </div>
1	D	257	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8416 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.

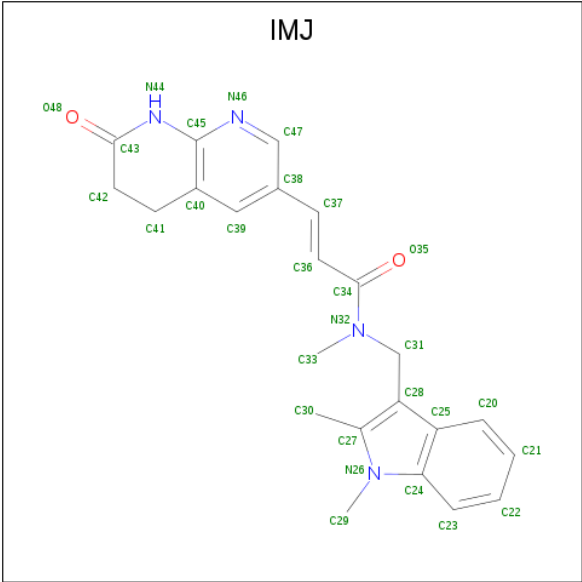
- Molecule 1 is a protein called Enoyl-[acyl-carrier-protein] reductase (FabL) (NADPH).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1958	1223	348	380	7			
1	D	256	Total	C	N	O	S	0	0	0
			1950	1218	347	379	6			
1	B	256	Total	C	N	O	S	0	0	0
			1950	1218	347	379	6			
1	C	256	Total	C	N	O	S	0	0	0
			1950	1218	347	379	6			

There are 4 discrepancies between the modelled and reference sequences:

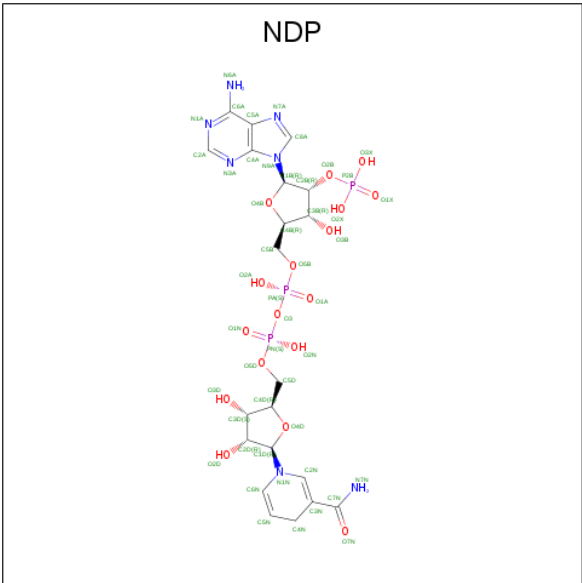
Chain	Residue	Modelled	Actual	Comment	Reference
A	257	LEU	-	EXPRESSION TAG	UNP Q81GI3
D	257	LEU	-	EXPRESSION TAG	UNP Q81GI3
B	257	LEU	-	EXPRESSION TAG	UNP Q81GI3
C	257	LEU	-	EXPRESSION TAG	UNP Q81GI3

- Molecule 2 is (2E)-N-[(1,2-dimethyl-1H-indol-3-yl)methyl]-N-methyl-3-(7-oxo-5,6,7,8-tetrahydro-1,8-naphthyridin-3-yl)prop-2-enamide (three-letter code: IMJ) (formula: C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	23	4	2		
2	D	1	Total	C	N	O	0	0
			29	23	4	2		
2	B	1	Total	C	N	O	0	0
			29	23	4	2		
2	C	1	Total	C	N	O	0	0
			29	23	4	2		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

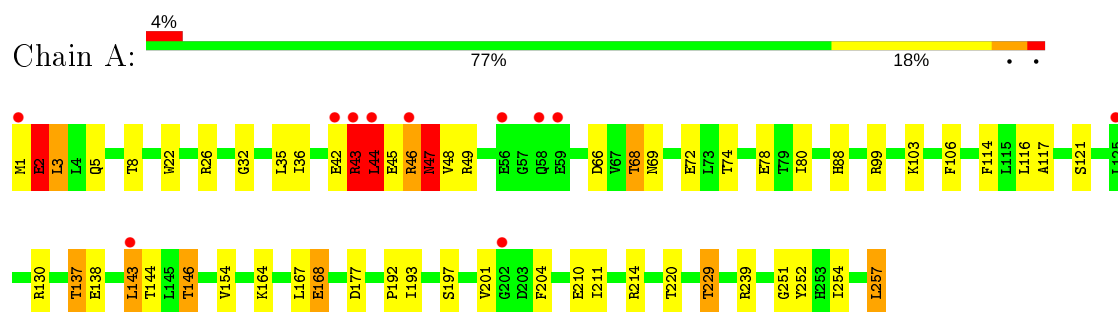
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	D	86	Total	O	0	0
			86	86		
4	B	79	Total	O	0	0
			79	79		
4	C	62	Total	O	0	0
			62	62		

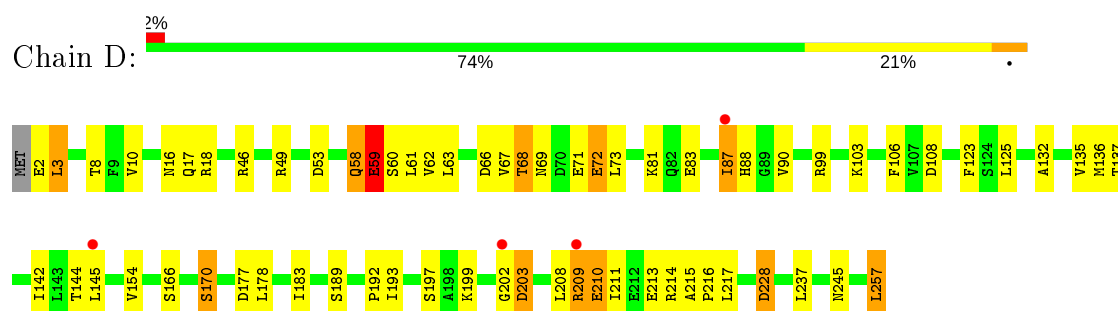
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

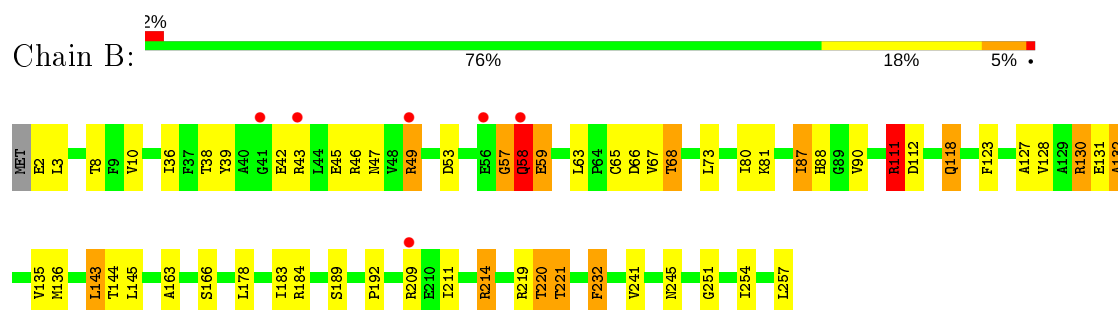
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase (FabL) (NADPH)



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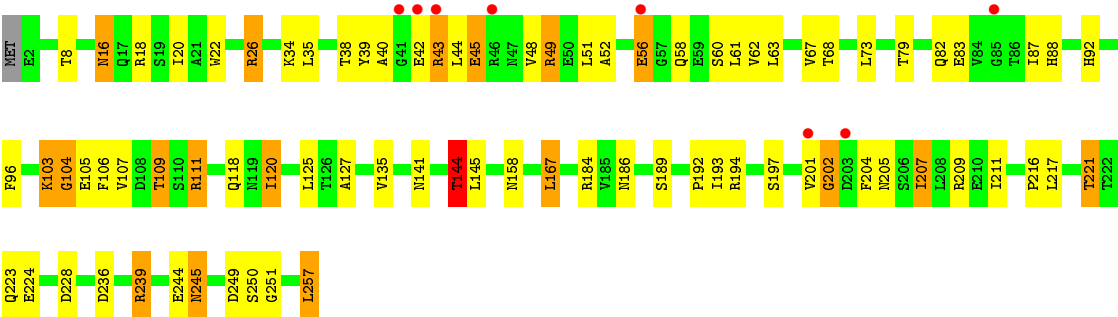


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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.74 Å 89.26 Å 185.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.20 29.59 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.59-2.20) 95.5 (29.59-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.20 Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.183 , 0.225 0.182 , 0.218	Depositor DCC
$R_{free}$ test set	3044 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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, IMJ

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	0.98	2/1983 (0.1%)	0.96	3/2678 (0.1%)
1	B	1.01	2/1975 (0.1%)	0.96	2/2668 (0.1%)
1	C	0.99	0/1975	0.96	3/2668 (0.1%)
1	D	1.09	2/1975 (0.1%)	0.96	6/2668 (0.2%)
All	All	1.02	6/7908 (0.1%)	0.96	14/10682 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	2
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	ALA	CA-CB	5.59	1.64	1.52
1	D	90	VAL	CB-CG2	5.46	1.64	1.52
1	A	168	GLU	CB-CG	5.22	1.62	1.52
1	B	232	PHE	CE2-CZ	5.22	1.47	1.37
1	D	166	SER	CB-OG	-5.08	1.35	1.42
1	A	239	ARG	CG-CD	5.00	1.64	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	LEU	CA-CB-CG	6.02	129.16	115.30
1	D	49	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	184	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	116	LEU	CA-CB-CG	5.50	127.94	115.30
1	D	59	GLU	CB-CA-C	5.49	121.38	110.40
1	B	221	THR	N-CA-CB	5.41	120.58	110.30
1	D	46	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	C	144	THR	CB-CA-C	-5.38	97.08	111.60
1	A	130	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	D	53	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	44	LEU	CA-CB-CG	5.20	127.25	115.30
1	D	108	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	228	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	257	LEU	CB-CG-CD1	-5.13	102.28	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	ARG	Peptide
1	B	219	ARG	Peptide
1	B	57	GLY	Peptide
1	B	58	GLN	Peptide
1	C	202	GLY	Peptide
1	C	56	GLU	Peptide

## 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	1958	0	1963	43	0
1	B	1950	0	1951	39	0
1	C	1950	0	1951	72	0
1	D	1950	0	1951	53	0
2	A	29	0	24	2	0
2	B	29	0	24	2	0
2	C	29	0	24	2	0
2	D	29	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	26	4	0
3	B	48	0	26	2	0
3	C	48	0	26	5	0
3	D	48	0	26	4	0
4	A	73	0	0	1	0
4	B	79	0	0	1	0
4	C	62	0	0	2	0
4	D	86	0	0	0	0
All	All	8416	0	8016	196	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 12.

All (196) 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:D:87:ILE:HD11	1:D:135:VAL:CG2	1.56	1.33
1:C:236:ASP:O	1:C:239:ARG:HG2	1.42	1.19
1:B:67:VAL:HA	1:B:73:LEU:HD21	1.35	1.08
1:D:87:ILE:CD1	1:D:135:VAL:CG2	2.36	1.03
1:D:87:ILE:HD11	1:D:135:VAL:HG21	1.04	1.02
1:D:87:ILE:CD1	1:D:135:VAL:HG23	1.94	0.98
1:D:132:ALA:HB1	1:D:136:MET:HE2	1.45	0.95
1:A:146:THR:HG23	1:A:167:LEU:HD23	1.51	0.90
1:B:65:CYS:SG	1:B:73:LEU:HD23	2.12	0.90
1:B:131:GLU:O	1:B:132:ALA:HB3	1.70	0.90
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.34	0.90
1:D:87:ILE:HD11	1:D:135:VAL:HG23	1.52	0.88
1:C:8:THR:H	1:C:88:HIS:HD2	1.18	0.87
1:C:236:ASP:O	1:C:239:ARG:CG	2.23	0.87
1:C:221:THR:HB	4:C:317:HOH:O	1.76	0.85
1:A:69:ASN:HD22	1:A:72:GLU:H	1.26	0.82
1:A:146:THR:HG21	1:A:168:GLU:HG3	1.60	0.81
1:D:63:LEU:HD12	1:D:63:LEU:N	1.93	0.81
1:B:131:GLU:O	1:B:132:ALA:CB	2.29	0.80
1:D:2:GLU:O	1:D:3:LEU:HB2	1.80	0.80
1:D:136:MET:HE3	1:D:142:ILE:HD11	1.64	0.79
1:B:143:LEU:C	1:B:143:LEU:HD23	2.02	0.79
1:B:39:TYR:CZ	1:B:45:GLU:HG3	2.20	0.77
1:C:96:PHE:HB3	1:C:120:ILE:HD12	1.68	0.76
1:D:132:ALA:HB1	1:D:136:MET:CE	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:THR:H	1:D:88:HIS:HD2	1.35	0.74
1:A:66:ASP:OD1	1:A:68:THR:HB	1.85	0.74
1:D:61:LEU:HB3	1:D:63:LEU:HD11	1.69	0.73
1:C:92:HIS:ND1	1:C:144:THR:HG23	2.04	0.72
1:C:106:PHE:O	1:C:109:THR:HG23	1.91	0.71
1:B:143:LEU:HD23	1:B:144:THR:N	2.06	0.69
1:A:143:LEU:HD22	1:A:144:THR:H	1.58	0.69
1:B:66:ASP:OD1	1:B:68:THR:HB	1.92	0.69
1:D:2:GLU:O	1:D:3:LEU:CB	2.41	0.68
1:C:22:TRP:O	1:C:26:ARG:HG2	1.94	0.68
1:A:46:ARG:O	1:A:47:ASN:HB2	1.95	0.67
1:C:87:ILE:HG12	1:C:135:VAL:HG13	1.77	0.66
1:C:192:PRO:HG2	1:C:211:ILE:HD11	1.77	0.66
1:D:62:VAL:C	1:D:63:LEU:HD12	2.16	0.66
1:B:220:THR:HG23	4:B:258:HOH:O	1.94	0.66
1:C:106:PHE:O	1:C:109:THR:CG2	2.44	0.66
1:C:144:THR:HG21	1:C:167:LEU:HD11	1.78	0.65
1:A:146:THR:HG22	1:A:164:LYS:HD2	1.79	0.65
1:A:214:ARG:HH12	1:A:257:LEU:HD11	1.62	0.65
1:C:96:PHE:CB	1:C:120:ILE:HD12	2.25	0.65
1:C:16:ASN:C	1:C:16:ASN:HD22	2.00	0.64
1:D:193:ILE:H	3:D:502:NDP:H72N	1.45	0.64
2:C:804:IMJ:H33B	3:C:504:NDP:C3N	2.27	0.64
1:B:132:ALA:O	1:B:136:MET:HG3	1.98	0.63
1:A:44:LEU:HD21	3:A:501:NDP:O1X	1.99	0.63
1:A:36:ILE:HD13	1:A:80:ILE:HD12	1.79	0.63
1:B:65:CYS:SG	1:B:73:LEU:CD2	2.86	0.63
1:B:132:ALA:HA	1:B:135:VAL:HG12	1.81	0.62
1:A:8:THR:H	1:A:88:HIS:HD2	1.47	0.62
1:A:192:PRO:HA	3:A:501:NDP:H71N	1.66	0.61
1:C:103:LYS:O	1:C:104:GLY:O	2.19	0.60
1:D:132:ALA:CB	1:D:136:MET:HE2	2.26	0.60
1:A:8:THR:H	1:A:88:HIS:CD2	2.20	0.59
1:D:132:ALA:CB	1:D:136:MET:CE	2.80	0.59
1:B:214:ARG:CG	1:B:214:ARG:HH11	2.12	0.59
1:A:197:SER:O	2:A:801:IMJ:H39	2.01	0.59
1:A:2:GLU:HA	1:A:5:GLN:HB2	1.85	0.59
1:D:136:MET:CE	1:D:142:ILE:HD11	2.30	0.58
1:C:8:THR:H	1:C:88:HIS:CD2	2.09	0.58
1:D:63:LEU:N	1:D:63:LEU:CD1	2.65	0.58
1:A:22:TRP:NE1	1:A:26:ARG:HD2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:THR:H	1:B:88:HIS:HD2	1.50	0.58
1:C:194:ARG:NH1	1:C:205:ASN:OD1	2.38	0.57
1:D:210:GLU:OE2	1:D:214:ARG:HD3	2.04	0.57
1:D:189:SER:HB2	1:D:245:ASN:HD21	1.69	0.56
1:D:192:PRO:HA	3:D:502:NDP:H71N	1.71	0.56
1:D:228:ASP:OD2	1:C:239:ARG:NH1	2.26	0.55
1:C:73:LEU:HD21	1:C:127:ALA:HB1	1.88	0.55
1:C:144:THR:HG21	1:C:167:LEU:HD21	1.88	0.55
1:C:16:ASN:C	1:C:16:ASN:ND2	2.60	0.55
1:C:197:SER:O	2:C:804:IMJ:H39	2.07	0.55
1:C:16:ASN:ND2	1:C:18:ARG:H	2.05	0.54
1:D:16:ASN:HD21	1:D:18:ARG:HH21	1.55	0.54
1:B:130:ARG:HB3	1:C:107:VAL:HG22	1.89	0.54
1:D:69:ASN:CG	1:D:72:GLU:HB2	2.28	0.54
1:C:141:ASN:HD21	1:C:186:ASN:HD22	1.55	0.53
1:D:69:ASN:ND2	1:D:72:GLU:HB2	2.24	0.53
1:A:177:ASP:OD2	1:D:106:PHE:HB3	2.09	0.52
1:D:144:THR:OG1	1:D:145:LEU:N	2.41	0.52
1:A:3:LEU:C	1:A:3:LEU:HD23	2.30	0.52
1:B:118:GLN:HE22	1:B:166:SER:CB	2.23	0.52
1:C:184:ARG:HD3	1:C:239:ARG:O	2.10	0.52
1:A:146:THR:HG21	1:A:168:GLU:CG	2.37	0.51
1:A:74:THR:O	1:A:78:GLU:HB2	2.09	0.51
1:A:192:PRO:HA	3:A:501:NDP:N7N	2.26	0.51
1:C:244:GLU:HG3	1:C:245:ASN:N	2.25	0.51
1:C:38:THR:HA	1:C:63:LEU:O	2.11	0.51
1:A:36:ILE:HG21	1:A:80:ILE:CD1	2.41	0.51
1:D:192:PRO:HA	3:D:502:NDP:N7N	2.26	0.50
1:C:58:GLN:OE1	1:C:58:GLN:HA	2.11	0.50
1:A:42:GLU:O	1:A:45:GLU:HB2	2.12	0.50
1:B:128:VAL:O	1:B:131:GLU:O	2.30	0.50
1:B:251:GLY:O	1:B:254:ILE:HG12	2.12	0.50
1:C:42:GLU:O	1:C:44:LEU:N	2.43	0.50
1:D:10:VAL:HG23	1:D:87:ILE:HG21	1.94	0.50
1:B:36:ILE:HD12	1:B:87:ILE:HD11	1.95	0.49
1:B:49:ARG:NH2	1:B:53:ASP:OD1	2.45	0.49
1:C:144:THR:HG22	1:C:145:LEU:N	2.27	0.49
1:B:192:PRO:HD2	1:B:211:ILE:HD13	1.93	0.49
1:B:38:THR:HA	1:B:63:LEU:O	2.12	0.49
1:C:141:ASN:ND2	1:C:186:ASN:HD22	2.10	0.49
1:A:252:TYR:CE2	1:C:257:LEU:HD23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LEU:HD21	1:C:79:THR:HG21	1.94	0.49
1:D:213:GLU:HG3	1:D:214:ARG:HD2	1.94	0.49
1:C:96:PHE:CB	1:C:120:ILE:CD1	2.91	0.48
1:D:154:VAL:HG22	1:B:257:LEU:HD23	1.95	0.48
1:A:143:LEU:HD22	1:A:144:THR:N	2.26	0.48
1:A:192:PRO:HD2	1:A:211:ILE:HD13	1.95	0.48
1:A:214:ARG:NH1	1:A:257:LEU:HD11	2.27	0.48
1:A:229:THR:HB	1:B:232:PHE:CZ	2.48	0.48
2:B:803:IMJ:H30	3:B:503:NDP:H71N	1.79	0.48
1:C:192:PRO:HA	3:C:504:NDP:H71N	1.79	0.48
1:B:214:ARG:NH1	1:B:214:ARG:HG3	2.15	0.47
1:B:118:GLN:HG3	1:C:118:GLN:HG3	1.96	0.47
1:B:8:THR:H	1:B:88:HIS:CD2	2.32	0.47
1:A:137:THR:HG22	1:A:138:GLU:HG3	1.97	0.46
1:B:57:GLY:O	1:B:58:GLN:HB3	2.16	0.46
1:B:143:LEU:C	1:B:143:LEU:CD2	2.76	0.46
1:C:40:ALA:HB2	3:C:504:NDP:C2A	2.46	0.46
1:D:58:GLN:O	1:D:59:GLU:O	2.33	0.46
1:C:20:ILE:HG21	1:C:145:LEU:HD13	1.96	0.46
1:C:184:ARG:CD	1:C:239:ARG:O	2.64	0.46
1:D:87:ILE:CG1	1:D:135:VAL:HG23	2.44	0.46
1:C:141:ASN:HA	1:C:184:ARG:O	2.15	0.46
1:C:217:LEU:HB2	1:C:250:SER:HB3	1.98	0.46
1:A:154:VAL:HG11	2:A:801:IMJ:H29A	1.97	0.46
1:D:87:ILE:HD12	1:D:135:VAL:HG23	1.91	0.45
1:A:44:LEU:O	1:A:48:VAL:HG23	2.16	0.45
1:D:199:LYS:O	1:D:199:LYS:HG3	2.16	0.45
1:D:192:PRO:HD2	1:D:211:ILE:HD13	1.98	0.45
1:B:189:SER:HB2	1:B:245:ASN:HD21	1.82	0.45
1:D:66:ASP:OD1	1:D:68:THR:HB	2.16	0.45
1:C:201:VAL:HG12	4:C:306:HOH:O	2.17	0.45
1:A:106:PHE:HB3	1:D:177:ASP:OD2	2.17	0.44
1:B:80:ILE:HG21	1:B:87:ILE:HD13	1.98	0.44
1:C:49:ARG:NH2	1:C:60:SER:O	2.44	0.44
1:C:34:LYS:C	1:C:35:LEU:HD12	2.38	0.44
1:C:42:GLU:C	1:C:44:LEU:H	2.19	0.44
1:A:43:ARG:HA	1:A:45:GLU:H	1.82	0.44
1:C:204:PHE:O	1:C:207:ILE:HG13	2.17	0.44
1:D:125:LEU:HD23	1:D:170:SER:OG	2.18	0.44
1:C:51:LEU:O	1:C:52:ALA:C	2.56	0.43
1:A:251:GLY:O	1:A:254:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PHE:CE2	1:C:111:ARG:HB2	2.53	0.43
1:C:189:SER:HB2	1:C:245:ASN:HD21	1.83	0.43
1:A:69:ASN:ND2	1:A:72:GLU:H	2.05	0.43
1:C:201:VAL:HG22	1:C:202:GLY:H	1.84	0.43
1:C:216:PRO:HG2	1:C:251:GLY:HA3	2.00	0.43
1:A:117:ALA:O	1:A:121:SER:HB2	2.19	0.43
1:C:44:LEU:O	1:C:45:GLU:C	2.57	0.43
2:B:803:IMJ:H33B	3:B:503:NDP:C3N	2.49	0.43
1:D:192:PRO:HG2	1:D:211:ILE:HD11	2.00	0.42
1:A:1:MET:HB2	1:A:32:GLY:CA	2.49	0.42
1:C:144:THR:CG2	1:C:167:LEU:HD11	2.47	0.42
1:C:236:ASP:OD1	1:C:239:ARG:HD3	2.18	0.42
1:A:114:PHE:CD1	1:D:123:PHE:HB2	2.55	0.42
1:D:197:SER:HB3	2:D:802:IMJ:H36	2.00	0.42
1:B:10:VAL:HB	1:B:90:VAL:HG22	2.02	0.42
1:C:193:ILE:H	3:C:504:NDP:H72N	1.65	0.42
1:C:26:ARG:NH2	1:C:224:GLU:OE2	2.52	0.42
1:B:111:ARG:NH1	1:C:67:VAL:O	2.35	0.42
1:D:209:ARG:HA	1:D:209:ARG:HD2	1.59	0.42
1:C:192:PRO:CG	1:C:211:ILE:HD11	2.48	0.42
1:C:20:ILE:HG21	1:C:145:LEU:CD1	2.50	0.42
1:D:217:LEU:HD21	1:C:184:ARG:HG2	2.01	0.42
1:D:208:LEU:HD12	1:D:208:LEU:HA	1.84	0.42
1:D:81:LYS:HB2	1:D:135:VAL:CG1	2.50	0.42
1:D:237:LEU:HA	1:C:228:ASP:HB3	2.02	0.42
1:C:221:THR:HG21	1:C:249:ASP:HA	2.02	0.42
1:C:96:PHE:HB3	1:C:120:ILE:CD1	2.44	0.42
1:B:43:ARG:H	1:B:43:ARG:HG3	1.62	0.41
1:C:40:ALA:HB2	3:C:504:NDP:N3A	2.36	0.41
1:A:103:LYS:HE2	1:A:103:LYS:HB3	1.65	0.41
1:C:125:LEU:HD22	1:C:144:THR:OG1	2.21	0.41
1:C:39:TYR:CE1	1:C:62:VAL:HG12	2.56	0.41
1:A:193:ILE:H	3:A:501:NDP:H72N	1.65	0.41
1:A:36:ILE:HG21	1:A:80:ILE:HD11	2.01	0.41
1:B:123:PHE:CE2	1:B:127:ALA:HB2	2.56	0.41
1:A:220:THR:HB	4:A:260:HOH:O	2.21	0.41
1:C:144:THR:HG22	1:C:145:LEU:H	1.85	0.41
1:C:39:TYR:HB3	1:C:48:VAL:HG21	2.03	0.41
1:D:215:ALA:O	1:D:216:PRO:C	2.57	0.41
1:A:201:VAL:HG21	1:A:204:PHE:HD1	1.86	0.41
1:B:178:LEU:HB3	1:B:183:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:PRO:HD2	1:C:211:ILE:CD1	2.52	0.40
1:D:67:VAL:HG22	3:D:502:NDP:N1A	2.35	0.40
1:C:35:LEU:HD12	1:C:35:LEU:N	2.36	0.40
1:D:178:LEU:HB3	1:D:183:ILE:HB	2.02	0.40
1:B:111:ARG:NH1	1:C:68:THR:HA	2.36	0.40
1:D:87:ILE:CG1	1:D:135:VAL:CG2	2.97	0.40
1:D:257:LEU:HA	1:D:257:LEU:HD23	1.92	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	255/257 (99%)	238 (93%)	14 (6%)	3 (1%)	13	10
1	B	254/257 (99%)	238 (94%)	12 (5%)	4 (2%)	9	7
1	C	254/257 (99%)	232 (91%)	17 (7%)	5 (2%)	7	4
1	D	254/257 (99%)	239 (94%)	9 (4%)	6 (2%)	6	3
All	All	1017/1028 (99%)	947 (93%)	52 (5%)	18 (2%)	8	5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	LEU
1	A	47	ASN
1	D	59	GLU
1	C	43	ARG
1	C	104	GLY
1	C	105	GLU
1	D	3	LEU

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Mol	Chain	Res	Type
1	D	58	GLN
1	D	202	GLY
1	B	59	GLU
1	B	132	ALA
1	C	56	GLU
1	D	60	SER
1	B	111	ARG
1	B	221	THR
1	D	203	ASP
1	C	158	ASN

### 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	206/206 (100%)	191 (93%)	15 (7%)	14	15
1	B	205/206 (100%)	184 (90%)	21 (10%)	7	6
1	C	205/206 (100%)	185 (90%)	20 (10%)	8	7
1	D	205/206 (100%)	190 (93%)	15 (7%)	14	15
All	All	821/824 (100%)	750 (91%)	71 (9%)	10	10

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	35	LEU
1	A	43	ARG
1	A	44	LEU
1	A	46	ARG
1	A	47	ASN
1	A	49	ARG
1	A	68	THR
1	A	99	ARG
1	A	137	THR
1	A	143	LEU

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Mol	Chain	Res	Type
1	A	146	THR
1	A	210	GLU
1	A	229	THR
1	A	257	LEU
1	D	17	GLN
1	D	68	THR
1	D	71	GLU
1	D	72	GLU
1	D	73	LEU
1	D	83	GLU
1	D	87	ILE
1	D	99	ARG
1	D	103	LYS
1	D	137	THR
1	D	170	SER
1	D	203	ASP
1	D	209	ARG
1	D	210	GLU
1	D	257	LEU
1	B	2	GLU
1	B	3	LEU
1	B	42	GLU
1	B	46	ARG
1	B	47	ASN
1	B	49	ARG
1	B	58	GLN
1	B	59	GLU
1	B	68	THR
1	B	81	LYS
1	B	87	ILE
1	B	111	ARG
1	B	112	ASP
1	B	118	GLN
1	B	130	ARG
1	B	143	LEU
1	B	145	LEU
1	B	209	ARG
1	B	214	ARG
1	B	220	THR
1	B	241	VAL
1	C	16	ASN
1	C	26	ARG

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Mol	Chain	Res	Type
1	C	43	ARG
1	C	45	GLU
1	C	49	ARG
1	C	61	LEU
1	C	82	GLN
1	C	83	GLU
1	C	103	LYS
1	C	109	THR
1	C	111	ARG
1	C	120	ILE
1	C	144	THR
1	C	167	LEU
1	C	207	ILE
1	C	209	ARG
1	C	221	THR
1	C	223	GLN
1	C	239	ARG
1	C	245	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	29	HIS
1	A	47	ASN
1	A	69	ASN
1	A	88	HIS
1	A	98	ASN
1	D	30	ASN
1	D	88	HIS
1	D	245	ASN
1	B	47	ASN
1	B	88	HIS
1	B	118	GLN
1	B	245	ASN
1	C	16	ASN
1	C	47	ASN
1	C	88	HIS
1	C	98	ASN
1	C	141	ASN
1	C	245	ASN
1	C	253	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	$\# Z  > 2$
3	NDP	D	502	-	45,52,52	1.48	6 (13%)	53,80,80	1.70	9 (16%)
3	NDP	C	504	-	45,52,52	1.76	5 (11%)	53,80,80	1.55	8 (15%)
3	NDP	B	503	-	45,52,52	1.58	6 (13%)	53,80,80	1.68	10 (18%)
2	IMJ	B	803	-	29,32,32	3.64	16 (55%)	36,46,46	2.71	15 (41%)
2	IMJ	D	802	-	29,32,32	3.38	14 (48%)	36,46,46	2.90	14 (38%)
2	IMJ	C	804	-	29,32,32	3.50	13 (44%)	36,46,46	3.11	17 (47%)
3	NDP	A	501	-	45,52,52	1.58	8 (17%)	53,80,80	1.45	5 (9%)
2	IMJ	A	801	-	29,32,32	4.04	15 (51%)	36,46,46	2.59	15 (41%)

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
3	NDP	D	502	-	-	9/30/77/77	0/5/5/5
3	NDP	C	504	-	-	9/30/77/77	0/5/5/5
3	NDP	B	503	-	-	8/30/77/77	0/5/5/5
2	IMJ	B	803	-	-	0/11/22/22	0/4/4/4
2	IMJ	D	802	-	-	0/11/22/22	0/4/4/4
2	IMJ	C	804	-	-	0/11/22/22	0/4/4/4
3	NDP	A	501	-	-	7/30/77/77	0/5/5/5
2	IMJ	A	801	-	-	0/11/22/22	0/4/4/4

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	IMJ	C40-C45	9.54	1.50	1.41
2	A	801	IMJ	C21-C20	9.48	1.58	1.36
2	B	803	IMJ	C21-C20	9.09	1.57	1.36
2	A	801	IMJ	C22-C23	8.70	1.56	1.36
2	D	802	IMJ	C22-C23	8.46	1.56	1.36
2	C	804	IMJ	C40-C45	7.88	1.49	1.41
3	C	504	NDP	O7N-C7N	7.70	1.42	1.24
2	D	802	IMJ	C21-C20	7.25	1.53	1.36
2	A	801	IMJ	C39-C38	7.06	1.51	1.39
2	C	804	IMJ	C39-C38	6.69	1.51	1.39
2	C	804	IMJ	C22-C23	6.66	1.51	1.36
2	D	802	IMJ	C39-C38	6.66	1.51	1.39
2	B	803	IMJ	C40-C45	6.46	1.47	1.41
2	B	803	IMJ	C41-C40	-6.33	1.40	1.51
2	B	803	IMJ	C22-C23	6.22	1.50	1.36
3	A	501	NDP	O7N-C7N	5.95	1.38	1.24
2	C	804	IMJ	C41-C40	-5.94	1.41	1.51
2	C	804	IMJ	C27-C28	5.92	1.51	1.39
2	C	804	IMJ	C21-C20	5.92	1.50	1.36
2	B	803	IMJ	C27-C28	5.85	1.51	1.39
2	D	802	IMJ	C40-C45	5.57	1.46	1.41
2	B	803	IMJ	C39-C38	5.54	1.49	1.39
3	B	503	NDP	O7N-C7N	5.42	1.37	1.24
3	D	502	NDP	O7N-C7N	5.39	1.37	1.24
3	C	504	NDP	C6N-C5N	5.21	1.42	1.33
2	A	801	IMJ	C20-C25	-5.10	1.31	1.42
2	C	804	IMJ	C20-C25	-4.88	1.32	1.42
2	D	802	IMJ	C41-C40	-4.65	1.43	1.51
2	D	802	IMJ	C20-C25	-4.49	1.33	1.42
2	A	801	IMJ	C41-C40	-4.45	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	IMJ	C27-N26	-4.39	1.35	1.39
2	B	803	IMJ	C27-N26	-4.32	1.35	1.39
2	D	802	IMJ	C27-C28	4.28	1.48	1.39
3	D	502	NDP	P2B-O2B	4.18	1.67	1.59
3	C	504	NDP	C2A-N3A	4.06	1.38	1.32
2	A	801	IMJ	C43-N44	4.05	1.39	1.35
2	A	801	IMJ	C27-C28	4.05	1.47	1.39
2	B	803	IMJ	C23-C24	-4.02	1.33	1.41
2	B	803	IMJ	C39-C40	3.94	1.46	1.39
2	D	802	IMJ	C39-C40	3.93	1.46	1.39
3	B	503	NDP	C2A-N1A	3.92	1.41	1.33
2	C	804	IMJ	C45-N44	-3.90	1.33	1.38
2	A	801	IMJ	C39-C40	3.75	1.45	1.39
3	A	501	NDP	C6N-C5N	3.61	1.39	1.33
3	B	503	NDP	C2A-N3A	3.56	1.37	1.32
2	A	801	IMJ	C23-C24	-3.51	1.34	1.41
2	B	803	IMJ	C33-N32	-3.44	1.33	1.45
3	B	503	NDP	C6N-C5N	3.42	1.39	1.33
2	C	804	IMJ	C33-N32	-3.35	1.34	1.45
2	B	803	IMJ	C20-C25	-3.33	1.35	1.42
2	C	804	IMJ	C23-C24	-3.26	1.34	1.41
2	C	804	IMJ	C39-C40	3.18	1.44	1.39
2	D	802	IMJ	C27-N26	-3.17	1.36	1.39
2	A	801	IMJ	C33-N32	-3.12	1.35	1.45
2	D	802	IMJ	C33-N32	-2.99	1.35	1.45
3	D	502	NDP	C6N-C5N	2.99	1.38	1.33
3	A	501	NDP	P2B-O2B	2.98	1.64	1.59
3	A	501	NDP	C2A-N3A	2.91	1.36	1.32
2	D	802	IMJ	C23-C24	-2.86	1.35	1.41
3	D	502	NDP	C2A-N3A	2.84	1.36	1.32
3	A	501	NDP	C2A-N1A	2.77	1.39	1.33
2	B	803	IMJ	C45-N44	-2.74	1.34	1.38
2	B	803	IMJ	C36-C34	2.71	1.52	1.48
2	C	804	IMJ	C41-C42	-2.65	1.45	1.52
2	B	803	IMJ	C41-C42	-2.60	1.45	1.52
3	B	503	NDP	C2N-C3N	2.59	1.42	1.34
2	B	803	IMJ	C22-C21	-2.58	1.31	1.38
3	A	501	NDP	C2N-C3N	2.53	1.42	1.34
2	B	803	IMJ	C34-N32	2.50	1.38	1.35
2	C	804	IMJ	C27-N26	-2.49	1.37	1.39
3	D	502	NDP	C2A-N1A	2.49	1.38	1.33
2	A	801	IMJ	O48-C43	2.47	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	504	NDP	C2A-N1A	2.44	1.38	1.33
2	A	801	IMJ	C31-C28	-2.32	1.49	1.51
2	D	802	IMJ	C31-C28	2.31	1.52	1.51
3	B	503	NDP	P2B-O2B	2.25	1.63	1.59
3	C	504	NDP	C2N-C3N	2.25	1.41	1.34
2	D	802	IMJ	C29-N26	2.24	1.52	1.47
2	D	802	IMJ	C22-C21	-2.09	1.32	1.38
3	A	501	NDP	PN-O2N	-2.08	1.45	1.55
3	D	502	NDP	C4N-C3N	2.08	1.54	1.49
3	A	501	NDP	PN-O1N	-2.06	1.43	1.50
2	A	801	IMJ	C42-C43	2.01	1.54	1.50

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	IMJ	C42-C43-N44	10.04	123.72	116.24
2	C	804	IMJ	C42-C43-N44	9.38	123.22	116.24
2	B	803	IMJ	C42-C43-N44	9.05	122.98	116.24
3	D	502	NDP	N3A-C2A-N1A	-7.77	116.54	128.68
2	A	801	IMJ	C42-C43-N44	6.81	121.31	116.24
3	B	503	NDP	N3A-C2A-N1A	-6.71	118.19	128.68
3	C	504	NDP	N3A-C2A-N1A	-5.98	119.33	128.68
2	D	802	IMJ	C20-C25-C28	-5.91	123.97	134.17
3	A	501	NDP	N3A-C2A-N1A	-5.88	119.49	128.68
2	B	803	IMJ	C38-C39-C40	-5.78	113.58	121.69
2	C	804	IMJ	C29-N26-C27	5.55	129.53	124.09
2	A	801	IMJ	C29-N26-C27	-5.34	118.86	124.09
2	B	803	IMJ	C42-C41-C40	5.27	123.22	112.03
2	D	802	IMJ	C38-C39-C40	-5.20	114.40	121.69
2	B	803	IMJ	N44-C45-N46	5.04	122.28	116.83
2	D	802	IMJ	C42-C41-C40	5.01	122.67	112.03
2	C	804	IMJ	C38-C39-C40	-4.86	114.87	121.69
2	C	804	IMJ	C21-C20-C25	4.84	127.61	120.89
2	C	804	IMJ	C22-C21-C20	-4.77	113.76	120.44
3	C	504	NDP	O4B-C1B-C2B	-4.61	98.60	106.59
2	A	801	IMJ	C38-C39-C40	-4.56	115.29	121.69
2	C	804	IMJ	O48-C43-N44	-4.56	117.41	121.43
2	C	804	IMJ	C42-C41-C40	4.54	121.67	112.03
2	D	802	IMJ	C21-C20-C25	-4.54	114.60	120.89
2	A	801	IMJ	N44-C45-N46	4.34	121.51	116.83
2	C	804	IMJ	C30-C27-N26	4.24	127.87	122.44
3	B	503	NDP	O7N-C7N-C3N	-3.97	113.41	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	803	IMJ	C39-C40-C45	3.88	121.61	116.87
2	A	801	IMJ	C36-C34-N32	3.85	120.89	118.00
2	A	801	IMJ	C47-N46-C45	3.83	123.75	116.05
2	A	801	IMJ	C23-C24-N26	-3.55	128.00	132.29
2	C	804	IMJ	C31-C28-C27	3.52	131.32	127.05
2	D	802	IMJ	C47-N46-C45	3.49	123.06	116.05
2	D	802	IMJ	C39-C38-C47	3.47	120.90	117.10
2	A	801	IMJ	C28-C27-N26	3.25	109.81	106.86
2	D	802	IMJ	N44-C45-N46	3.25	120.34	116.83
2	A	801	IMJ	C42-C41-C40	3.24	118.91	112.03
2	C	804	IMJ	C30-C27-C28	-3.16	122.41	129.24
2	C	804	IMJ	C28-C27-N26	3.11	109.68	106.86
3	B	503	NDP	C3N-C7N-N7N	3.09	123.15	117.67
2	C	804	IMJ	C23-C24-C25	-3.08	116.75	120.94
3	D	502	NDP	O4B-C1B-C2B	-3.06	101.28	106.59
2	C	804	IMJ	C47-N46-C45	3.04	122.16	116.05
3	B	503	NDP	C3N-C2N-N1N	-3.02	118.78	123.10
2	A	801	IMJ	C39-C40-C45	2.90	120.41	116.87
2	D	802	IMJ	O48-C43-N44	-2.79	118.97	121.43
2	C	804	IMJ	C22-C23-C24	2.79	124.79	119.44
2	C	804	IMJ	N44-C45-N46	2.76	119.81	116.83
3	A	501	NDP	O4D-C1D-N1N	2.73	113.39	108.06
2	A	801	IMJ	C37-C36-C34	-2.70	115.21	120.51
3	D	502	NDP	C1D-N1N-C6N	-2.69	115.03	120.83
2	B	803	IMJ	C30-C27-N26	2.68	125.87	122.44
3	B	503	NDP	C2A-N1A-C6A	2.68	123.33	118.75
2	A	801	IMJ	O48-C43-C42	-2.67	116.46	122.17
3	B	503	NDP	C1D-N1N-C6N	-2.67	115.08	120.83
3	D	502	NDP	C3N-C2N-N1N	-2.67	119.29	123.10
2	B	803	IMJ	C21-C20-C25	-2.66	117.21	120.89
3	C	504	NDP	C1D-N1N-C6N	-2.65	115.11	120.83
3	C	504	NDP	C4A-C5A-N7A	-2.63	106.66	109.40
3	B	503	NDP	O4B-C1B-C2B	-2.61	102.06	106.59
3	A	501	NDP	C3N-C7N-N7N	2.57	122.24	117.67
2	A	801	IMJ	C40-C45-N46	-2.57	118.44	122.44
3	C	504	NDP	O2B-P2B-O1X	-2.55	99.56	109.39
2	D	802	IMJ	C23-C24-C25	-2.53	117.49	120.94
2	D	802	IMJ	C31-N32-C34	2.53	126.27	119.96
2	C	804	IMJ	C39-C38-C47	2.52	119.87	117.10
2	A	801	IMJ	C45-N44-C43	-2.51	121.81	124.24
2	B	803	IMJ	C31-N32-C34	2.51	126.20	119.96
2	B	803	IMJ	C31-C28-C27	2.50	130.07	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	NDP	O4D-C4D-C3D	2.48	110.03	105.11
2	B	803	IMJ	C39-C38-C47	2.48	119.82	117.10
2	B	803	IMJ	C47-N46-C45	2.47	121.01	116.05
3	A	501	NDP	O2B-P2B-O1X	-2.44	99.96	109.39
3	D	502	NDP	C4D-O4D-C1D	-2.43	104.11	109.47
2	D	802	IMJ	C38-C47-N46	-2.43	121.53	124.21
2	B	803	IMJ	C29-N26-C27	2.42	126.46	124.09
2	B	803	IMJ	C23-C24-N26	-2.38	129.41	132.29
3	D	502	NDP	C2A-N1A-C6A	2.38	122.82	118.75
2	B	803	IMJ	O48-C43-C42	-2.36	117.12	122.17
2	D	802	IMJ	O48-C43-C42	-2.35	117.14	122.17
3	C	504	NDP	O2D-C2D-C3D	2.31	119.28	111.82
2	C	804	IMJ	C31-N32-C34	2.30	125.69	119.96
3	C	504	NDP	O4D-C1D-N1N	2.28	112.52	108.06
2	D	802	IMJ	C31-C28-C27	2.27	129.80	127.05
3	D	502	NDP	O2B-C2B-C1B	2.26	118.25	110.10
3	B	503	NDP	PN-O3-PA	-2.24	125.15	132.83
3	B	503	NDP	C5B-C4B-C3B	-2.20	106.93	115.18
3	C	504	NDP	O2N-PN-O1N	2.15	122.89	112.24
2	A	801	IMJ	C39-C38-C47	2.08	119.38	117.10
2	B	803	IMJ	C21-C22-C23	-2.07	117.54	120.44
3	A	501	NDP	O2D-C2D-C1D	2.05	116.89	110.02
3	B	503	NDP	C1B-N9A-C4A	-2.03	123.07	126.64
3	D	502	NDP	O2D-C2D-C1D	2.03	116.80	110.02

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	NDP	PN-O3-PA-O5B
3	D	502	NDP	C5D-O5D-PN-O1N
3	C	504	NDP	PN-O3-PA-O5B
3	C	504	NDP	C5D-O5D-PN-O1N
3	C	504	NDP	C5D-O5D-PN-O2N
3	B	503	NDP	PN-O3-PA-O5B
3	B	503	NDP	C5D-O5D-PN-O1N
3	B	503	NDP	C5D-O5D-PN-O2N
3	A	501	NDP	PN-O3-PA-O5B
3	A	501	NDP	C5D-O5D-PN-O1N
3	A	501	NDP	C5D-O5D-PN-O2N
3	C	504	NDP	C2B-O2B-P2B-O3X
3	C	504	NDP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	D	502	NDP	C5D-O5D-PN-O2N
3	B	503	NDP	O4D-C1D-N1N-C6N
3	A	501	NDP	O4D-C1D-N1N-C6N
3	C	504	NDP	O4D-C1D-N1N-C6N
3	D	502	NDP	C2D-C1D-N1N-C6N
3	D	502	NDP	O4D-C1D-N1N-C6N
3	C	504	NDP	C2D-C1D-N1N-C6N
3	B	503	NDP	C2D-C1D-N1N-C6N
3	A	501	NDP	C2D-C1D-N1N-C6N
3	D	502	NDP	O4B-C4B-C5B-O5B
3	D	502	NDP	C5D-O5D-PN-O3
3	B	503	NDP	C5D-O5D-PN-O3
3	A	501	NDP	C5D-O5D-PN-O3
3	D	502	NDP	C5B-O5B-PA-O1A
3	D	502	NDP	C5B-O5B-PA-O2A
3	C	504	NDP	C5B-O5B-PA-O1A
3	B	503	NDP	C2N-C3N-C7N-N7N
3	C	504	NDP	O4B-C4B-C5B-O5B
3	B	503	NDP	O4B-C4B-C5B-O5B
3	A	501	NDP	O4B-C4B-C5B-O5B

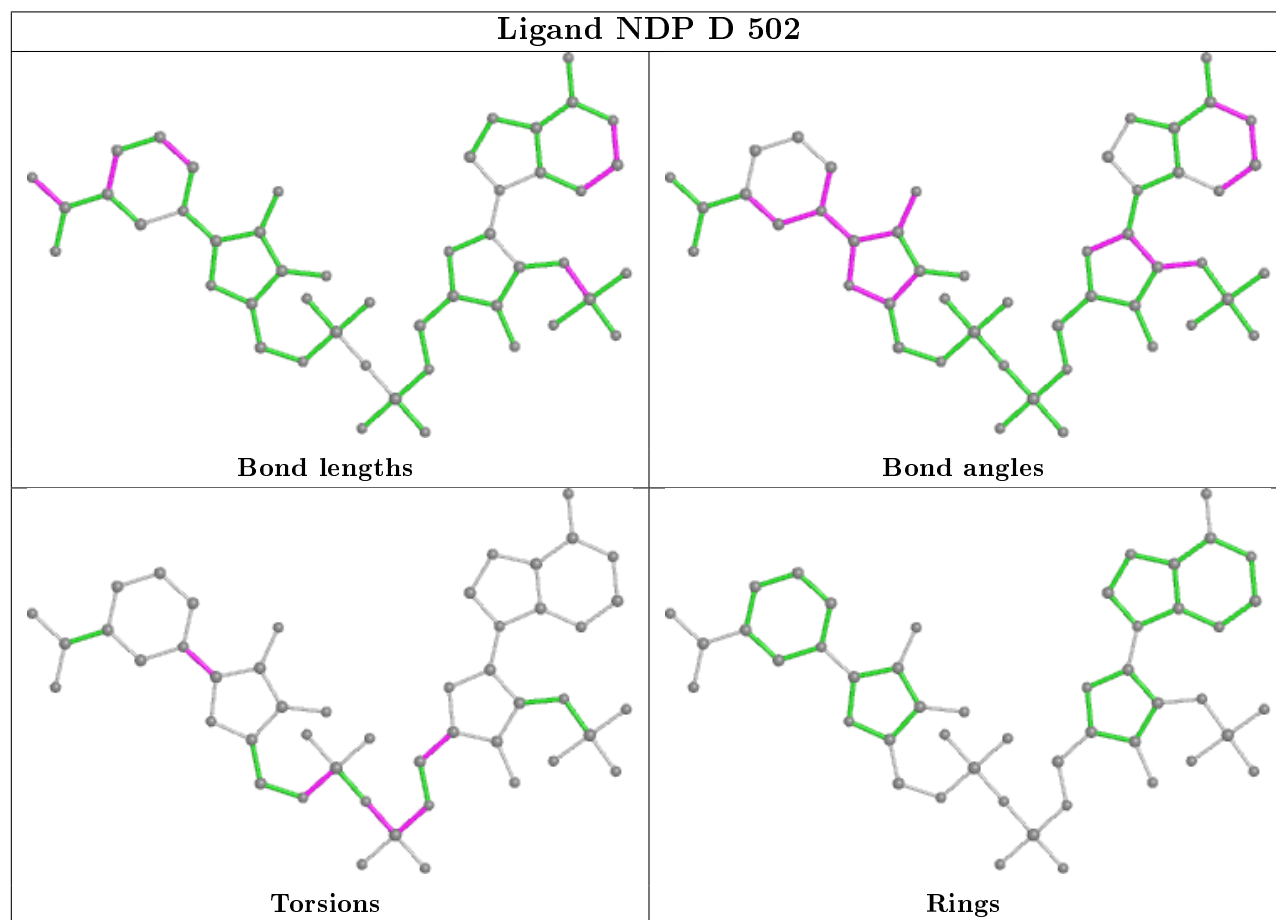
There are no ring outliers.

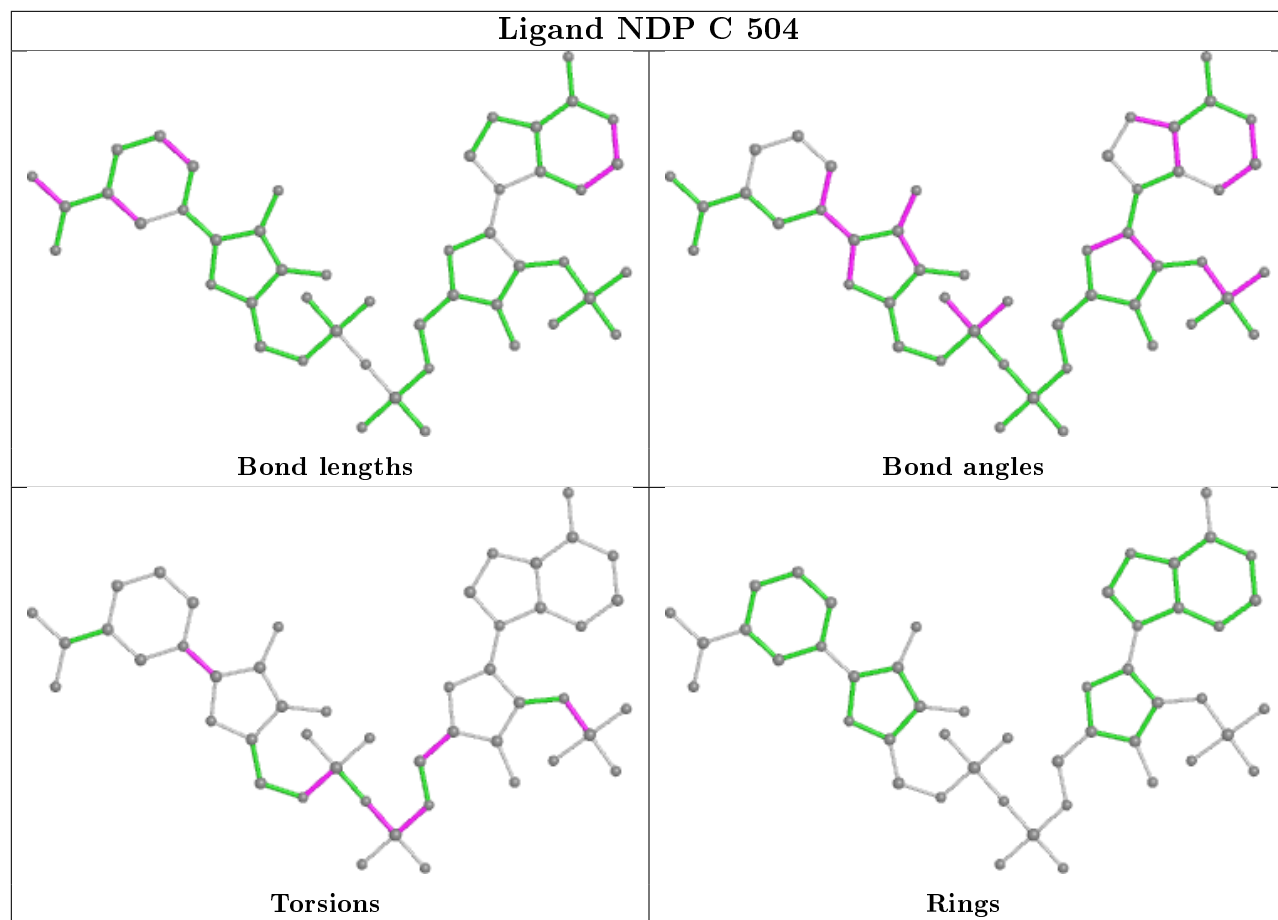
8 monomers are involved in 19 short contacts:

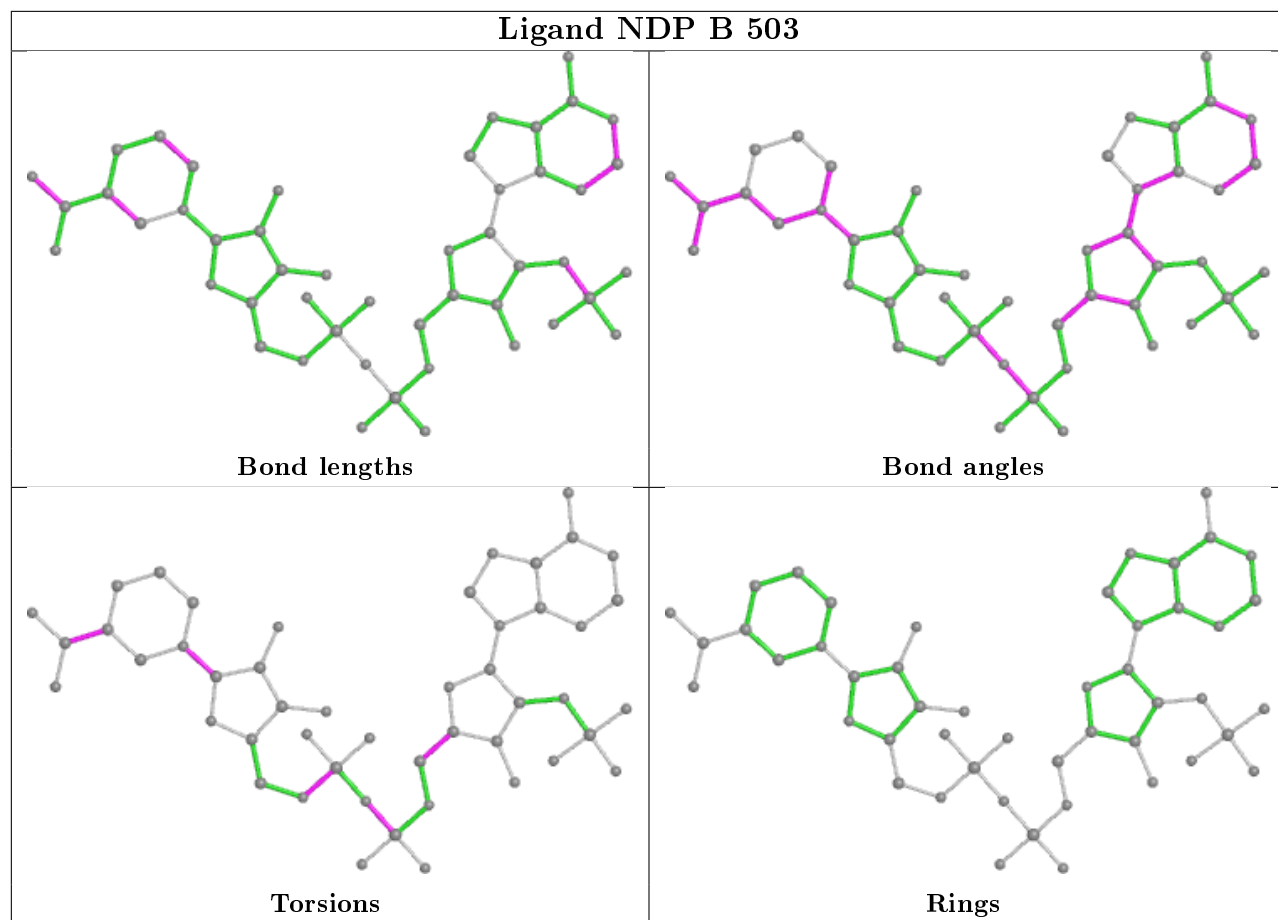
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	NDP	4	0
3	C	504	NDP	5	0
3	B	503	NDP	2	0
2	B	803	IMJ	2	0
2	D	802	IMJ	1	0
2	C	804	IMJ	2	0
3	A	501	NDP	4	0
2	A	801	IMJ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

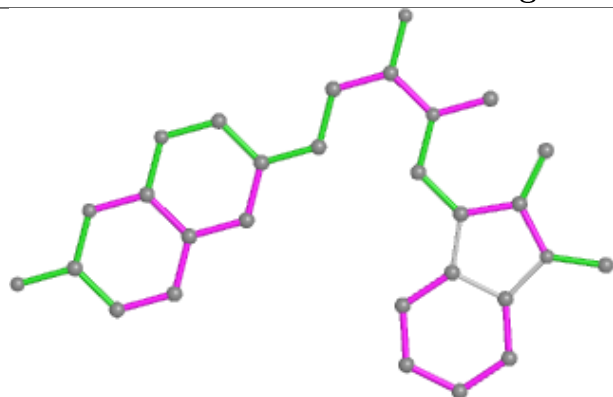
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



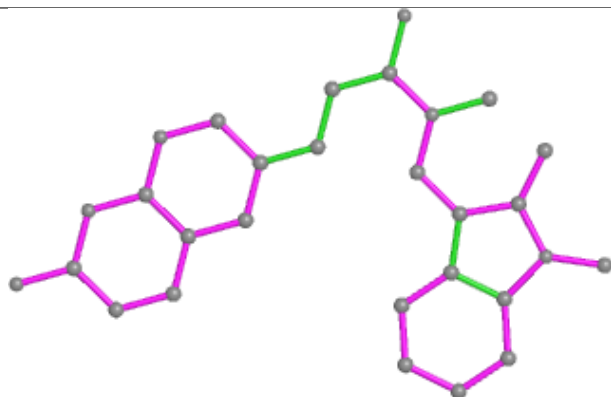




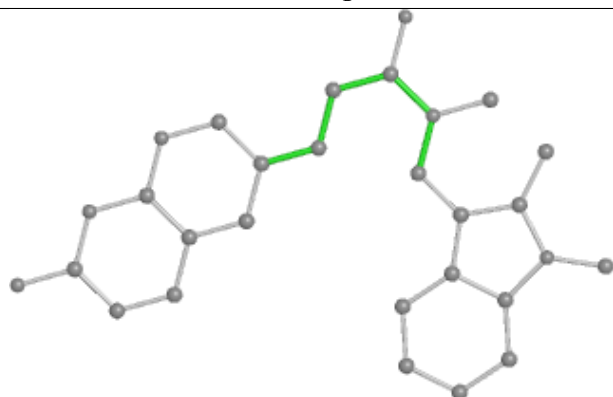
## Ligand IMJ B 803



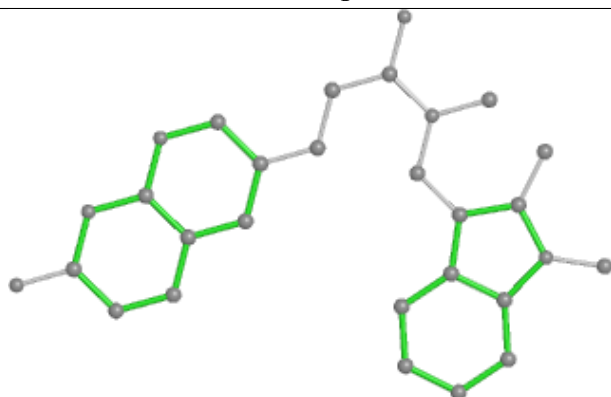
Bond lengths



Bond angles

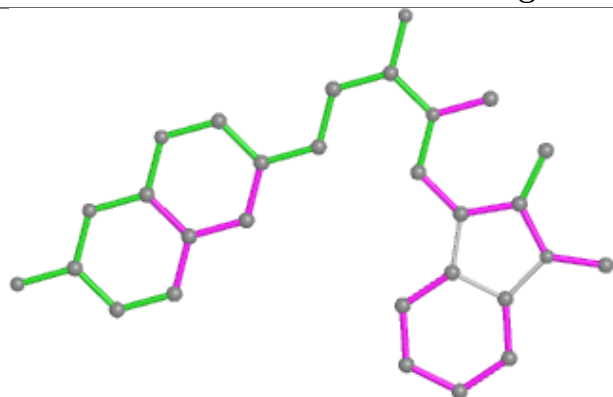


Torsions

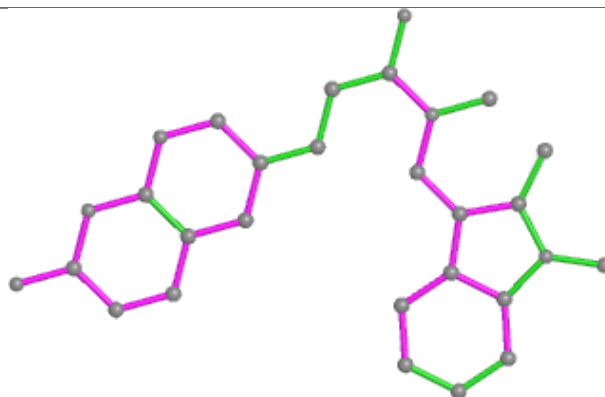


Rings

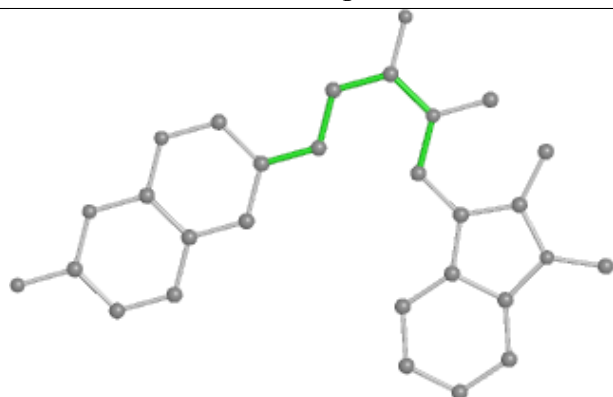
## Ligand IMJ D 802



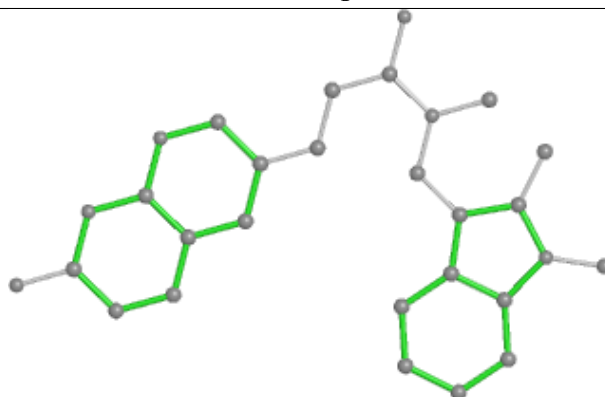
Bond lengths



Bond angles

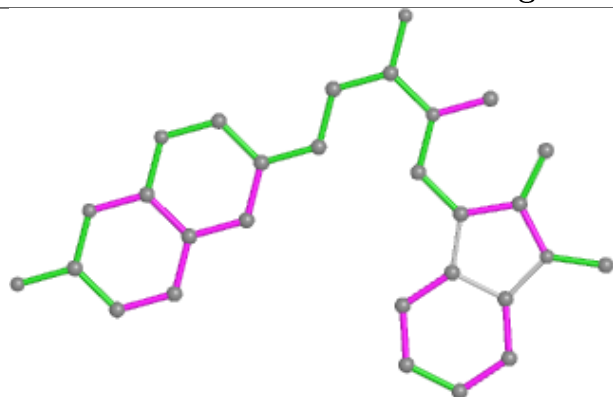


Torsions

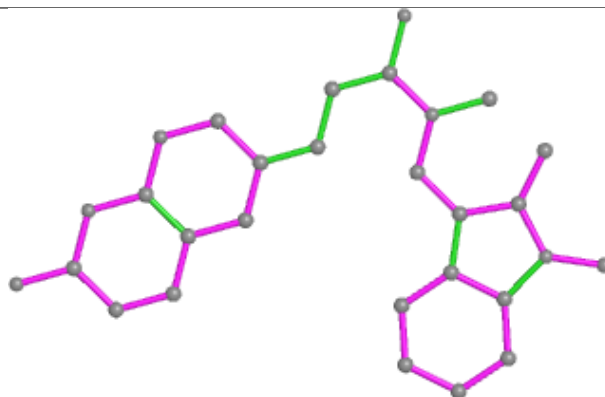


Rings

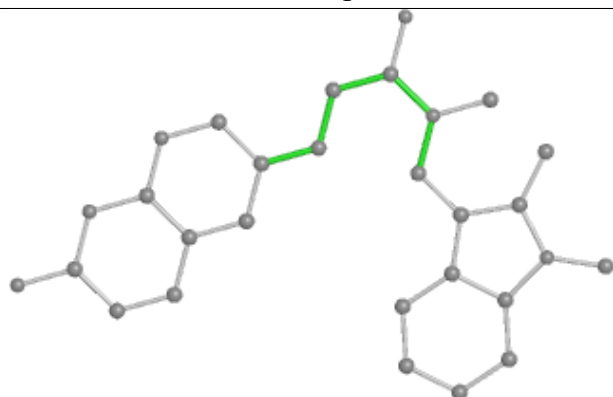
## Ligand IMJ C 804



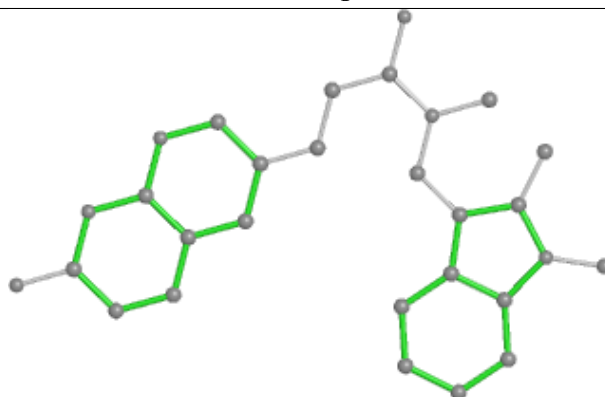
Bond lengths



Bond angles

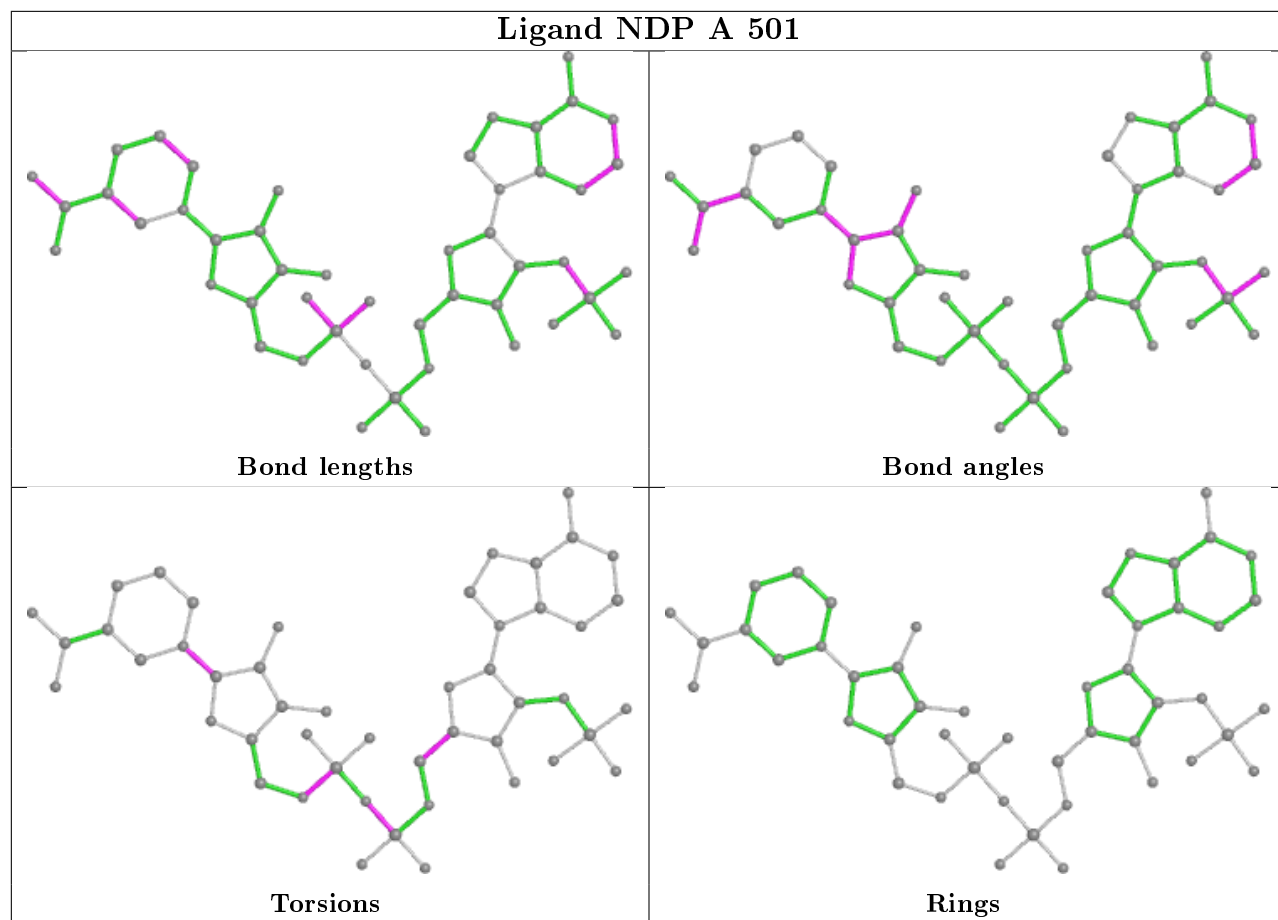


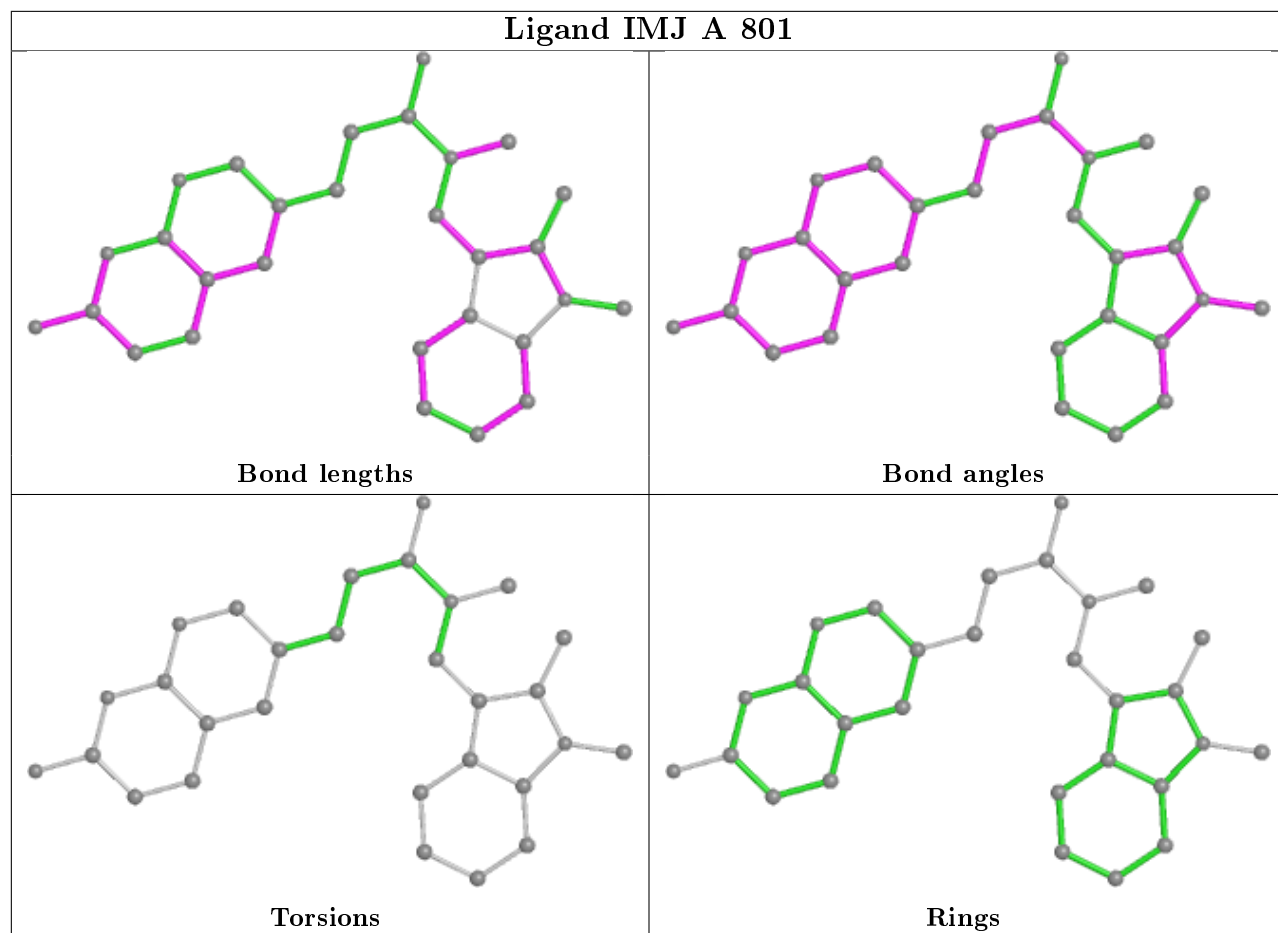
Torsions



Rings







## 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	257/257 (100%)	-0.39	11 (4%) 35 33	19, 32, 71, 98	0
1	B	256/257 (99%)	-0.29	6 (2%) 60 58	21, 34, 72, 106	0
1	C	256/257 (99%)	-0.19	8 (3%) 49 47	21, 37, 71, 102	0
1	D	256/257 (99%)	-0.47	4 (1%) 72 70	14, 28, 59, 77	0
All	All	1025/1028 (99%)	-0.34	29 (2%) 53 51	14, 33, 68, 106	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.4
1	C	46	ARG	4.2
1	C	43	ARG	3.8
1	A	46	ARG	3.7
1	B	56	GLU	3.6
1	B	41	GLY	3.2
1	C	201	VAL	3.1
1	A	56	GLU	3.1
1	C	56	GLU	2.9
1	A	44	LEU	2.8
1	B	43	ARG	2.7
1	A	58	GLN	2.7
1	D	202	GLY	2.6
1	B	58	GLN	2.5
1	A	143	LEU	2.5
1	A	59	GLU	2.5
1	A	43	ARG	2.5
1	B	209	ARG	2.5
1	A	202	GLY	2.4
1	D	87	ILE	2.4
1	A	125	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	49	ARG	2.3
1	C	203	ASP	2.3
1	A	42	GLU	2.3
1	C	85	GLY	2.3
1	D	209	ARG	2.1
1	D	145	LEU	2.1
1	C	42	GLU	2.0
1	C	41	GLY	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](#)

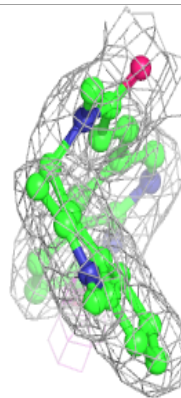
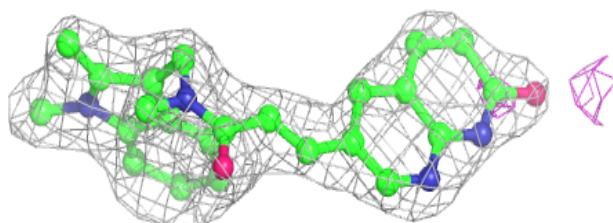
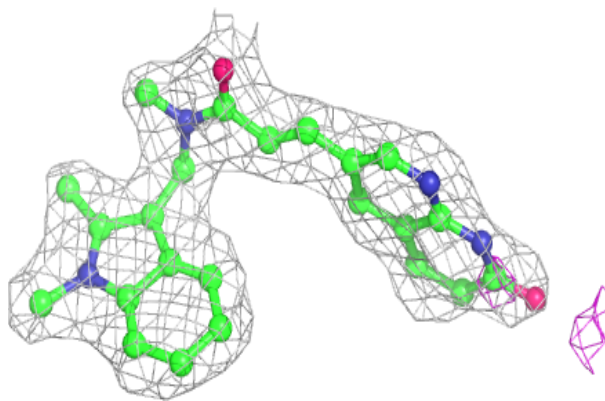
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IMJ	C	804	29/29	0.93	0.11	25,32,53,53	0
2	IMJ	A	801	29/29	0.95	0.10	22,26,33,34	0
2	IMJ	D	802	29/29	0.96	0.09	19,23,30,34	0
3	NDP	C	504	48/48	0.96	0.09	30,36,54,56	0
2	IMJ	B	803	29/29	0.96	0.09	23,31,39,41	0
3	NDP	D	502	48/48	0.97	0.10	24,28,30,35	0
3	NDP	A	501	48/48	0.97	0.09	28,31,46,48	0
3	NDP	B	503	48/48	0.97	0.10	19,33,45,46	0

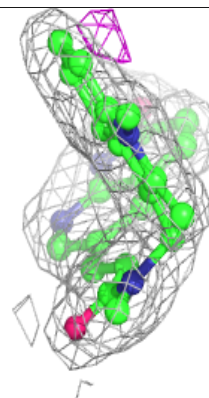
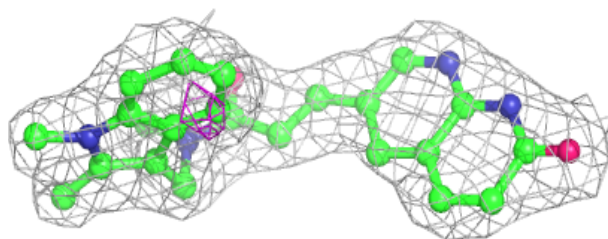
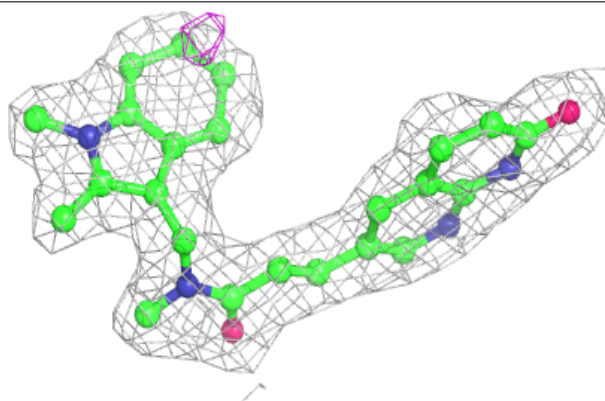
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around IMJ C 804:**

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

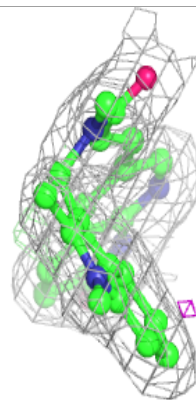
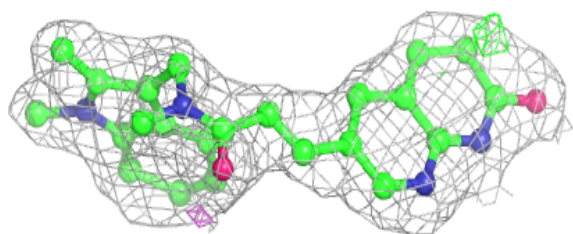
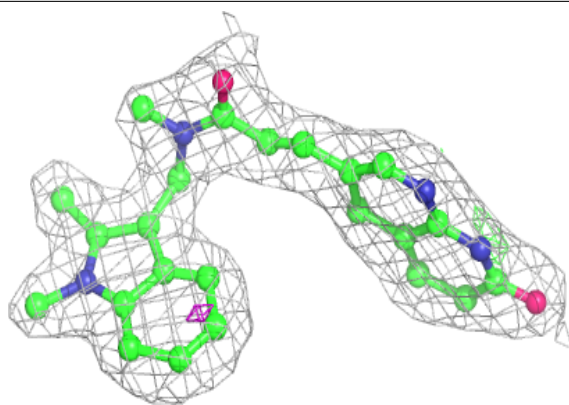
**Electron density around IMJ A 801:**

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

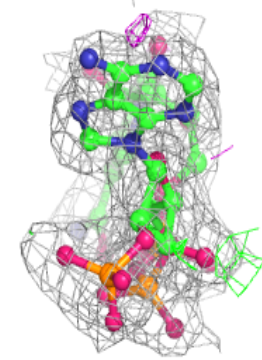
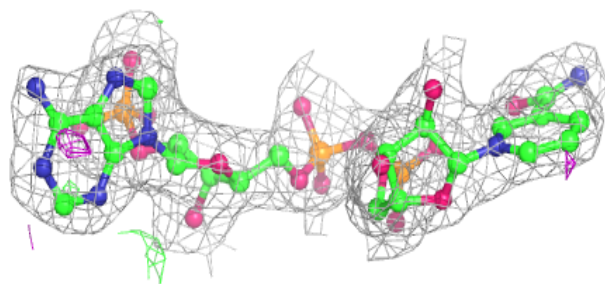
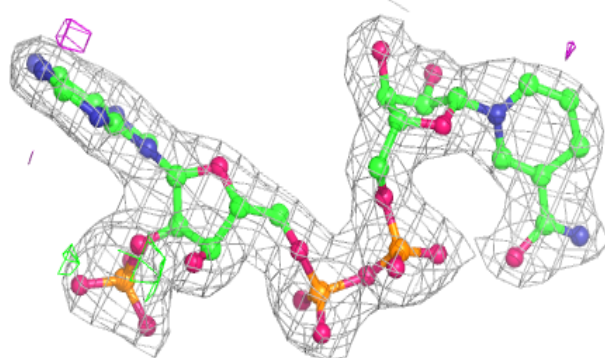


**Electron density around IMJ D 802:**

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

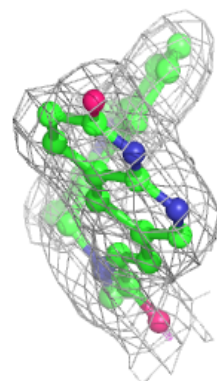
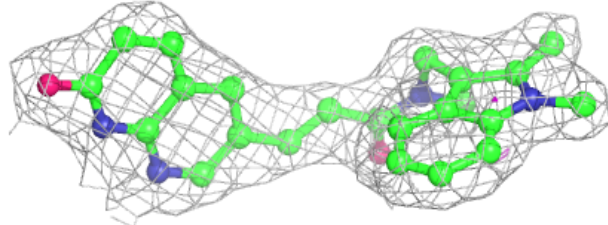
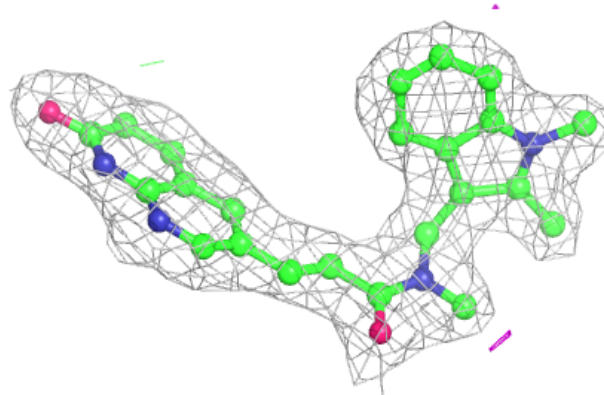
**Electron density around NDP C 504:**

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

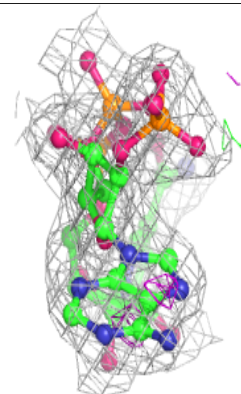
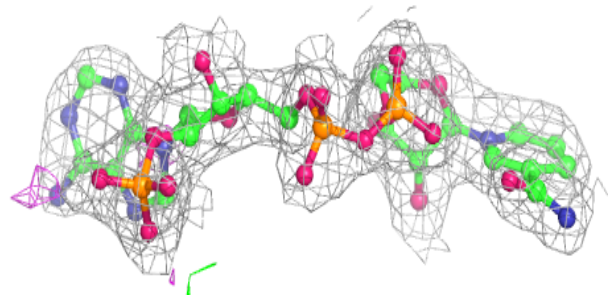
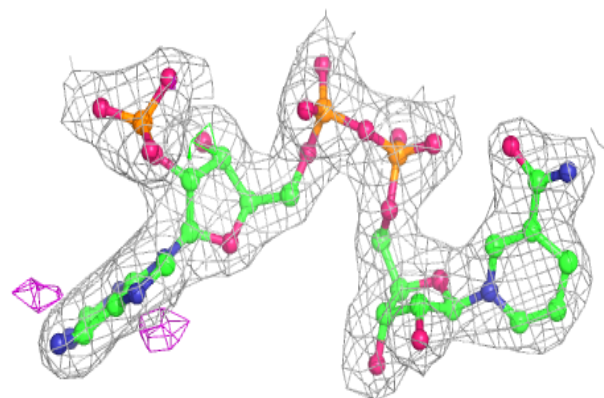


**Electron density around IMJ B 803:**

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

**Electron density around NDP D 502:**

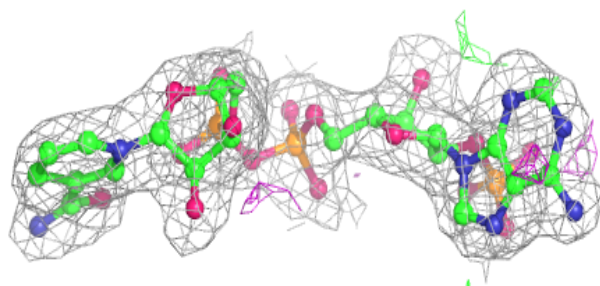
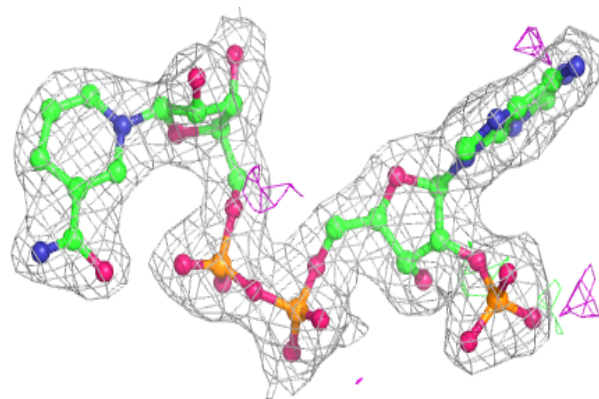
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



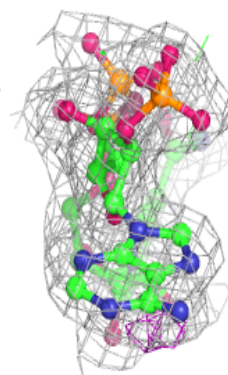
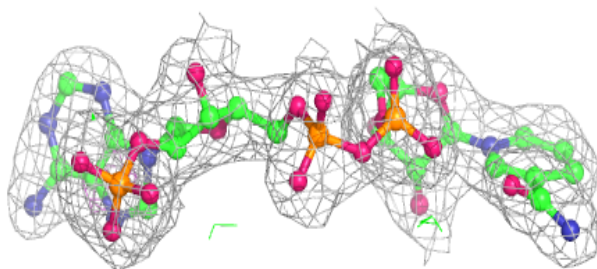
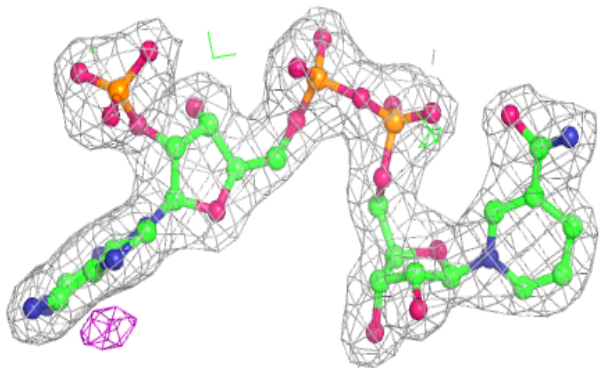


**Electron density around NDP A 501:**

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

**Electron density around NDP B 503:**

$2mF_o-DF_c$  (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.