



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:56 AM UTC

PDB ID : 6OWE / pdb_00006owe
Title : Enoyl-CoA carboxylases/reductases in complex with ethylmalonyl CoA
Authors : DeMirci, H.
Deposited on : 2019-05-09
Resolution : 1.72 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

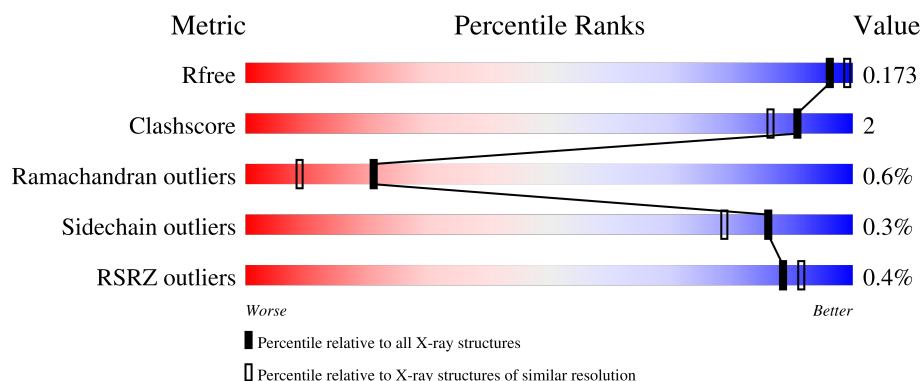
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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 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	449	95% 95% 95%
1	B	449	94% 94% 94%
1	C	449	98% 98% 98%
1	D	449	96% 96% 96%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15445 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.

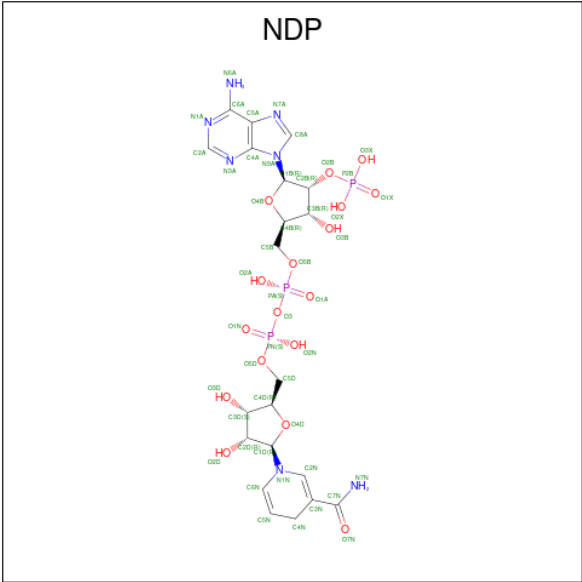
- Molecule 1 is a protein called Crotonyl-CoA carboxylase/reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	8	0
			3510	2202	634	661	13			
1	B	448	Total	C	N	O	S	0	7	0
			3517	2209	635	660	13			
1	C	447	Total	C	N	O	S	0	7	0
			3505	2199	636	656	14			
1	D	445	Total	C	N	O	S	0	6	0
			3477	2186	625	652	14			

There are 16 discrepancies between the modelled and reference sequences:

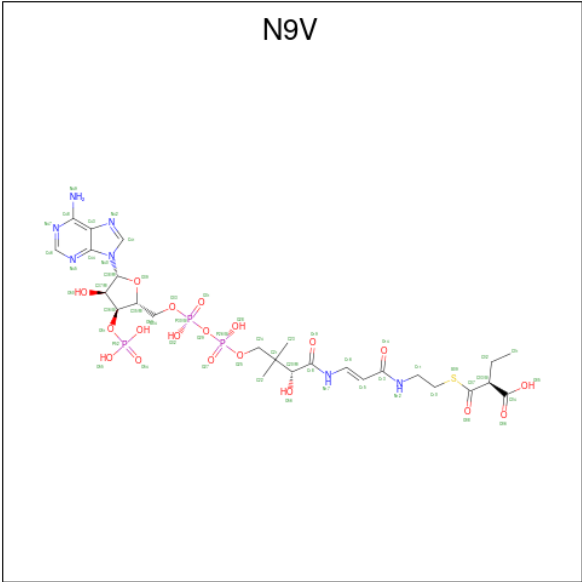
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP E4N096
A	-2	GLY	-	expression tag	UNP E4N096
A	-1	ARG	-	expression tag	UNP E4N096
A	0	HIS	-	expression tag	UNP E4N096
B	-3	GLU	-	expression tag	UNP E4N096
B	-2	GLY	-	expression tag	UNP E4N096
B	-1	ARG	-	expression tag	UNP E4N096
B	0	HIS	-	expression tag	UNP E4N096
C	-3	GLU	-	expression tag	UNP E4N096
C	-2	GLY	-	expression tag	UNP E4N096
C	-1	ARG	-	expression tag	UNP E4N096
C	0	HIS	-	expression tag	UNP E4N096
D	-3	GLU	-	expression tag	UNP E4N096
D	-2	GLY	-	expression tag	UNP E4N096
D	-1	ARG	-	expression tag	UNP E4N096
D	0	HIS	-	expression tag	UNP E4N096

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



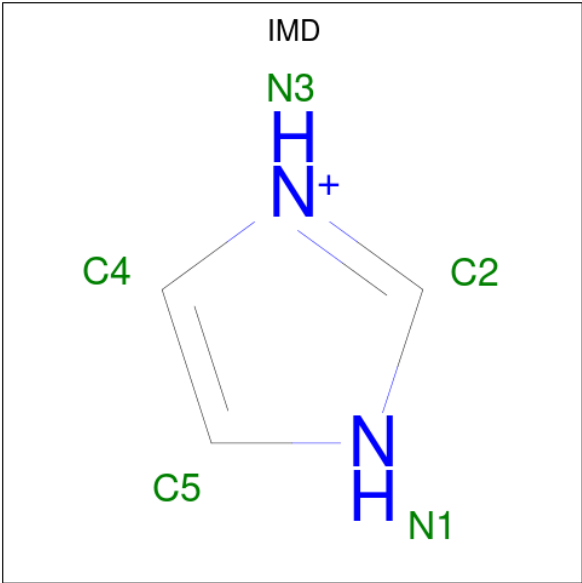
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5'-O-[(S)-{[(S)-[(3R)-4-({(1E)-3-[(2S)-2-carboxybutanoyl]sulfanyl}ethyl)amino]-3-oxoprop-1-en-1-yl}amino)-3-hydroxy-2,2-dimethyl-4-oxobutoxy](hydroxy)phosphoryl]oxy}{(hydroxy)phosphoryl]adenosine 3'-(dihydrogen phosphate) (CCD ID: N9V) (formula: C₂₆H₄₀N₇O₁₉P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			56	26	7	19	3	1		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	N	0	0
			5	3	2		
4	D	1	Total	C	N	0	0
			5	3	2		

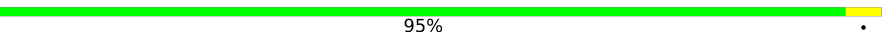
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	284	Total	O	0	0
			284	284		
5	B	307	Total	O	0	0
			307	307		
5	C	259	Total	O	0	0
			259	259		
5	D	262	Total	O	0	0
			262	262		

3 Residue-property plots [i](#)

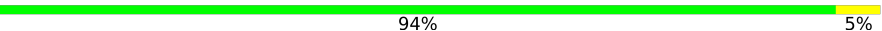
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

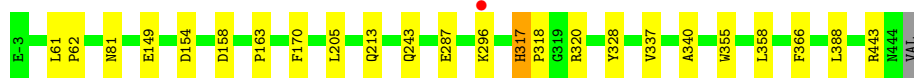
- Molecule 1: Crotonyl-CoA carboxylase/reductase

Chain A:  95%

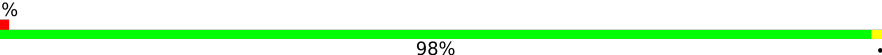


- Molecule 1: Crotonyl-CoA carboxylase/reductase

Chain B:  94%

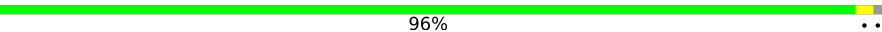


- Molecule 1: Crotonyl-CoA carboxylase/reductase

Chain C:  98%



- Molecule 1: Crotonyl-CoA carboxylase/reductase

Chain D:  96%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.10Å 78.70Å 138.90Å 90.00° 108.10° 90.00°	Depositor
Resolution (Å)	29.89 – 1.72 29.89 – 1.72	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.89-1.72) 97.2 (29.89-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 1.37Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472)	Depositor
R, R_{free}	0.157 , 0.170 0.159 , 0.173	Depositor DCC
R_{free} test set	1978 reflections (0.42%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15445	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4736e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, N9V, IMD

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	0.60	0/3592	0.68	0/4867
1	B	0.64	0/3599	0.70	0/4878
1	C	0.60	0/3587	0.69	0/4861
1	D	0.58	0/3559	0.68	0/4825
All	All	0.60	0/14337	0.69	0/19431

There are no bond length outliers.

There are no bond angle outliers.

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	3510	0	3432	14	0
1	B	3517	0	3446	15	0
1	C	3505	0	3430	4	0
1	D	3477	0	3406	6	0
2	A	48	0	23	2	0
2	B	48	0	23	2	0
2	C	48	0	24	1	0
2	D	48	0	23	2	0
3	A	56	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	56	0	0	5	0
4	A	5	0	5	1	0
4	B	5	0	5	1	0
4	C	5	0	5	2	0
4	D	5	0	5	3	0
5	A	284	0	0	3	0
5	B	307	0	0	2	0
5	C	259	0	0	0	0
5	D	262	0	0	2	0
All	All	15445	0	13827	47	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 2.

All (47) 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)
3:A:502:N9V:C02	5:A:722:HOH:O	2.30	0.80
3:A:502:N9V:C01	5:A:789:HOH:O	2.31	0.79
1:C:206:VAL:HG12	4:C:502:IMD:H5	1.76	0.67
1:B:170:PHE:CD2	3:D:501:N9V:O06	2.50	0.65
1:A:287[B]:GLU:H	1:A:287[B]:GLU:CD	2.07	0.61
1:B:317:HIS:H	1:B:318:PRO:CD	2.13	0.61
1:B:296[A]:LYS:HG2	1:B:328:TYR:OH	2.01	0.60
1:C:317:HIS:H	1:C:318:PRO:CD	2.19	0.56
1:A:287[B]:GLU:O	1:A:320[B]:ARG:NH1	2.37	0.56
1:D:317:HIS:H	1:D:318:PRO:CD	2.19	0.55
2:D:502:NDP:C6N	4:D:503:IMD:HN3	2.22	0.53
2:D:502:NDP:C6N	4:D:503:IMD:N3	2.72	0.53
1:A:205:LEU:HD21	2:A:501:NDP:H42N	1.90	0.53
5:B:720:HOH:O	3:D:501:N9V:C02	2.56	0.53
1:B:388:LEU:O	1:B:443:ARG:HD2	2.10	0.52
1:B:205:LEU:HD21	2:B:501:NDP:H42N	1.91	0.51
1:A:154:ASP:HB2	1:A:163:PRO:HD3	1.92	0.51
1:B:61:LEU:HD23	1:B:62:PRO:HD2	1.93	0.51
1:B:170:PHE:CE2	3:D:501:N9V:O06	2.65	0.50
1:A:317:HIS:H	1:A:318:PRO:CD	2.25	0.50
1:B:340:ALA:HB2	2:B:501:NDP:H1D	1.94	0.49
1:B:81:ASN:HD22	3:D:501:N9V:C02	2.25	0.49
1:A:170:PHE:CD2	3:A:502:N9V:O06	2.66	0.48
1:B:213:GLN:HG3	1:B:337:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:HB3	3:A:502:N9V:C01	2.44	0.48
4:D:503:IMD:H5	5:D:797:HOH:O	2.13	0.47
1:A:184:LYS:NZ	5:A:601:HOH:O	2.45	0.47
1:A:357:SER:HB2	1:A:359:LYS:HE3	1.95	0.47
1:B:243:GLN:CD	4:B:502:IMD:H4	2.40	0.47
1:D:49:ASP:HB3	1:D:52:LYS:HD2	1.96	0.47
1:A:81:ASN:ND2	3:A:502:N9V:C01	2.78	0.47
3:D:501:N9V:C01	5:D:728:HOH:O	2.61	0.47
1:B:154:ASP:HB2	1:B:163:PRO:HD3	1.97	0.47
1:B:287:GLU:O	1:B:320:ARG:NH2	2.50	0.44
1:C:337:VAL:HG12	1:C:362:VAL:HB	2.00	0.43
1:D:149:GLU:OE1	1:D:184:LYS:NZ	2.33	0.43
1:A:203:PRO:O	1:A:204:GLY:C	2.62	0.42
1:A:243:GLN:CD	4:A:503:IMD:H5	2.44	0.42
1:D:34:LYS:HE3	1:D:98:GLU:OE2	2.19	0.42
1:A:340:ALA:HB2	2:A:501:NDP:H1D	2.02	0.42
1:B:149:GLU:HG2	5:B:602:HOH:O	2.21	0.41
1:C:260:ARG:HD2	1:C:260:ARG:O	2.21	0.41
1:D:317:HIS:N	1:D:318:PRO:CD	2.84	0.41
1:A:213:GLN:HG3	1:A:337:VAL:HG22	2.03	0.41
1:B:317:HIS:N	1:B:318:PRO:CD	2.81	0.41
2:C:501:NDP:C6N	4:C:502:IMD:N1	2.84	0.40
1:D:213:GLN:HG2	1:D:315:PHE:CE2	2.57	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	453/449 (101%)	443 (98%)	7 (2%)	3 (1%)	18	7
1	B	454/449 (101%)	443 (98%)	8 (2%)	3 (1%)	18	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	452/449 (101%)	440 (97%)	10 (2%)	2 (0%)	30	16
1	D	449/449 (100%)	437 (97%)	10 (2%)	2 (0%)	30	16
All	All	1808/1796 (101%)	1763 (98%)	35 (2%)	10 (1%)	21	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	317	HIS
1	B	158	ASP
1	B	317	HIS
1	C	158	ASP
1	C	317	HIS
1	D	158	ASP
1	D	317	HIS
1	A	366	PHE
1	B	366	PHE

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	367/360 (102%)	366 (100%)	1 (0%)	86	79
1	B	367/360 (102%)	365 (100%)	2 (0%)	81	71
1	C	365/360 (101%)	364 (100%)	1 (0%)	86	79
1	D	363/360 (101%)	362 (100%)	1 (0%)	86	79
All	All	1462/1440 (102%)	1457 (100%)	5 (0%)	86	79

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

Mol	Chain	Res	Type
1	A	355	TRP
1	B	355	TRP

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Mol	Chain	Res	Type
1	B	358	LEU
1	C	355	TRP
1	D	355	TRP

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

Mol	Chain	Res	Type
1	A	410	GLN
1	B	157	ASN
1	B	351	ASN
1	B	399	GLN
1	C	81	ASN
1	C	207	ASN
1	C	218	ASN
1	C	288	HIS
1	C	289	HIS
1	C	351	ASN
1	C	406	HIS
1	D	207	ASN
1	D	289	HIS

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](#)

10 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
4	IMD	C	502	-	5,5,5	0.75	0	5,5,5	0.63	0
3	N9V	A	502	-	56,58,58	2.89	17 (30%)	74,86,86	1.97	15 (20%)
3	N9V	D	501	-	56,58,58	3.09	16 (28%)	74,86,86	2.20	16 (21%)
4	IMD	B	502	-	5,5,5	0.88	0	5,5,5	0.40	0
2	NDP	A	501	-	51,52,52	2.37	21 (41%)	71,80,80	1.28	8 (11%)
2	NDP	C	501	-	51,52,52	2.48	17 (33%)	71,80,80	1.36	11 (15%)
4	IMD	D	503	-	5,5,5	0.66	0	5,5,5	0.82	0
2	NDP	D	502	-	51,52,52	2.43	19 (37%)	71,80,80	1.33	10 (14%)
4	IMD	A	503	-	5,5,5	0.87	0	5,5,5	0.54	0
2	NDP	B	501	-	51,52,52	2.67	25 (49%)	71,80,80	1.23	5 (7%)

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
4	IMD	C	502	-	-	-	0/1/1/1
3	N9V	A	502	-	-	14/60/77/77	0/3/3/3
3	N9V	D	501	-	-	12/60/77/77	0/3/3/3
4	IMD	B	502	-	-	-	0/1/1/1
2	NDP	A	501	-	-	5/34/77/77	0/5/5/5
2	NDP	C	501	-	-	5/34/77/77	0/5/5/5
4	IMD	D	503	-	-	-	0/1/1/1
2	NDP	D	502	-	-	2/34/77/77	0/5/5/5
4	IMD	A	503	-	-	-	0/1/1/1
2	NDP	B	501	-	-	3/34/77/77	0/5/5/5

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	N9V	C03-C04	12.48	1.68	1.52
3	A	502	N9V	P52-O51	11.92	1.80	1.59
3	D	501	N9V	P52-O51	11.90	1.80	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NDP	P2B-O2B	9.05	1.75	1.59
2	D	502	NDP	P2B-O2B	9.00	1.75	1.59
2	B	501	NDP	P2B-O2B	8.79	1.74	1.59
3	A	502	N9V	C16-C15	7.19	1.58	1.36
3	A	502	N9V	C03-C07	-7.01	1.47	1.53
2	A	501	NDP	P2B-O2B	5.99	1.70	1.59
2	A	501	NDP	O4B-C4B	-5.96	1.31	1.45
2	C	501	NDP	O4B-C4B	-5.71	1.32	1.45
3	D	501	N9V	C16-C15	5.65	1.53	1.36
2	B	501	NDP	O2B-C2B	-5.63	1.24	1.44
3	D	501	N9V	C03-C07	-5.58	1.48	1.53
2	D	502	NDP	O4B-C4B	-5.42	1.33	1.45
3	A	502	N9V	C18-N17	5.40	1.42	1.34
3	A	502	N9V	C03-C04	5.24	1.58	1.52
2	C	501	NDP	O2B-C2B	-5.20	1.26	1.44
3	D	501	N9V	C18-N17	5.07	1.41	1.34
2	D	502	NDP	O2B-C2B	-5.05	1.26	1.44
2	C	501	NDP	O3B-C3B	-5.05	1.30	1.43
2	B	501	NDP	O3D-C3D	-4.82	1.31	1.43
3	D	501	N9V	P26-O29	-4.56	1.54	1.59
3	A	502	N9V	P26-O29	-4.53	1.54	1.59
2	A	501	NDP	O2B-C2B	-4.36	1.29	1.44
2	A	501	NDP	O5D-C5D	-4.35	1.28	1.44
2	A	501	NDP	O3B-C3B	-4.33	1.32	1.43
2	C	501	NDP	O3D-C3D	-4.30	1.32	1.43
2	B	501	NDP	O4B-C4B	-4.28	1.35	1.45
2	D	502	NDP	O3B-C3B	-4.25	1.32	1.43
2	B	501	NDP	O3B-C3B	-4.17	1.32	1.43
2	B	501	NDP	O5D-C5D	-3.94	1.29	1.44
2	B	501	NDP	PA-O3	3.82	1.63	1.59
2	D	502	NDP	C2B-C1B	3.68	1.62	1.53
2	A	501	NDP	PN-O5D	3.68	1.73	1.59
2	B	501	NDP	C3B-C2B	3.61	1.60	1.53
3	D	501	N9V	P30-O33	3.55	1.73	1.59
3	A	502	N9V	P30-O33	3.52	1.73	1.59
3	D	501	N9V	P26-O25	3.50	1.73	1.59
2	D	502	NDP	O3D-C3D	-3.49	1.34	1.43
2	C	501	NDP	C4N-C3N	-3.42	1.43	1.50
3	A	502	N9V	P26-O25	3.41	1.72	1.59
2	B	501	NDP	C4N-C3N	-3.40	1.43	1.50
2	A	501	NDP	O3D-C3D	-3.37	1.34	1.43
2	C	501	NDP	O5D-C5D	-3.36	1.31	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	NDP	C2A-N3A	-3.33	1.28	1.33
2	D	502	NDP	PA-O3	3.21	1.63	1.59
2	B	501	NDP	C2B-C1B	3.19	1.61	1.53
2	C	501	NDP	C2A-N3A	-3.19	1.28	1.33
3	A	502	N9V	C16-N17	3.14	1.49	1.40
2	B	501	NDP	C2A-N3A	-3.12	1.28	1.33
2	B	501	NDP	O7N-C7N	-3.04	1.17	1.24
3	A	502	N9V	C43-C44	3.03	1.44	1.39
2	C	501	NDP	C5D-C4D	3.01	1.60	1.51
3	D	501	N9V	C11-N12	-3.01	1.39	1.46
2	B	501	NDP	C5A-N7A	-2.98	1.33	1.39
2	D	502	NDP	PN-O3	-2.96	1.56	1.59
2	A	501	NDP	O2D-C2D	-2.96	1.35	1.43
3	A	502	N9V	C41-N42	2.92	1.37	1.31
3	A	502	N9V	O08-C07	-2.91	1.16	1.20
2	C	501	NDP	O4B-C1B	-2.90	1.35	1.42
3	A	502	N9V	O25-C24	-2.90	1.34	1.43
2	A	501	NDP	C3B-C2B	2.87	1.59	1.53
2	B	501	NDP	O2D-C2D	-2.85	1.35	1.43
2	A	501	NDP	C2B-C1B	2.84	1.60	1.53
2	B	501	NDP	O5B-C5B	-2.81	1.34	1.44
2	B	501	NDP	PN-O5D	2.81	1.70	1.59
2	B	501	NDP	C5B-C4B	2.79	1.60	1.51
2	A	501	NDP	PA-O2A	-2.77	1.42	1.55
2	B	501	NDP	P2B-O3X	-2.74	1.44	1.54
2	C	501	NDP	O4D-C4D	-2.74	1.38	1.45
2	A	501	NDP	O4D-C4D	-2.73	1.38	1.45
2	D	502	NDP	O2D-C2D	-2.73	1.36	1.43
2	D	502	NDP	O5D-C5D	-2.71	1.34	1.44
2	C	501	NDP	P2B-O3X	-2.71	1.44	1.54
2	A	501	NDP	C5A-N7A	-2.71	1.34	1.39
3	D	501	N9V	C16-N17	2.66	1.47	1.40
3	D	501	N9V	O51-C36	-2.66	1.35	1.44
2	A	501	NDP	O7N-C7N	-2.66	1.18	1.24
2	A	501	NDP	P2B-O3X	-2.65	1.44	1.54
2	A	501	NDP	PA-O1A	-2.65	1.41	1.50
2	D	502	NDP	P2B-O3X	-2.64	1.45	1.54
3	A	502	N9V	C07-S09	2.64	1.83	1.75
2	B	501	NDP	PA-O2A	-2.62	1.43	1.55
2	A	501	NDP	C2A-N3A	-2.60	1.29	1.33
3	D	501	N9V	C43-C44	2.55	1.43	1.39
3	D	501	N9V	O25-C24	-2.52	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	N9V	O19-C18	-2.52	1.18	1.23
3	A	502	N9V	O51-C36	-2.52	1.35	1.44
2	A	501	NDP	C4N-C5N	-2.52	1.42	1.49
3	D	501	N9V	C22-C21	-2.49	1.48	1.53
2	D	502	NDP	O4B-C1B	-2.46	1.36	1.42
2	D	502	NDP	C5B-C4B	2.45	1.58	1.51
2	C	501	NDP	PA-O2A	-2.44	1.44	1.55
2	D	502	NDP	PN-O5D	2.43	1.68	1.59
2	B	501	NDP	C6N-N1N	-2.41	1.31	1.37
2	D	502	NDP	PA-O1A	-2.39	1.42	1.50
2	B	501	NDP	PA-O1A	-2.38	1.42	1.50
2	B	501	NDP	O4D-C1D	-2.33	1.36	1.42
2	C	501	NDP	O2D-C2D	-2.30	1.37	1.43
2	A	501	NDP	C4N-C3N	-2.30	1.45	1.50
3	A	502	N9V	C13-N12	2.28	1.38	1.34
2	D	502	NDP	O4D-C4D	-2.26	1.40	1.45
2	B	501	NDP	C2D-C1D	2.23	1.60	1.53
2	D	502	NDP	PA-O2A	-2.23	1.45	1.55
2	A	501	NDP	O5B-C5B	-2.22	1.36	1.44
2	C	501	NDP	PN-O5D	2.20	1.68	1.59
2	B	501	NDP	C8A-N9A	-2.16	1.33	1.37
2	C	501	NDP	C5B-C4B	2.13	1.58	1.51
2	C	501	NDP	C2B-C1B	2.12	1.58	1.53
2	D	502	NDP	C5D-C4D	2.12	1.57	1.51
2	B	501	NDP	C2A-N1A	-2.10	1.30	1.33
2	A	501	NDP	C5D-C4D	2.10	1.57	1.51
3	D	501	N9V	C02-C03	-2.02	1.47	1.54
3	D	501	N9V	P30-O29	2.02	1.61	1.59

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	N9V	O08-C07-S09	-9.90	110.47	123.80
3	A	502	N9V	O08-C07-S09	-8.03	112.99	123.80
3	D	501	N9V	O08-C07-C03	7.12	135.31	124.11
3	A	502	N9V	O08-C07-C03	6.63	134.54	124.11
3	D	501	N9V	O28-P26-O29	5.12	121.12	107.27
3	A	502	N9V	O28-P26-O29	4.63	119.80	107.27
3	A	502	N9V	O19-C18-N17	-4.13	117.70	123.47
3	D	501	N9V	O19-C18-N17	-4.10	117.75	123.47
3	D	501	N9V	C23-C21-C20	4.07	115.71	108.77
2	C	501	NDP	O3-PA-O1A	-3.83	99.17	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	N9V	C10-C11-N12	-3.73	104.63	112.41
3	A	502	N9V	C23-C21-C20	3.45	114.65	108.77
2	A	501	NDP	C5A-C4A-N3A	-3.45	121.97	126.72
2	D	502	NDP	O3-PA-O1A	-3.41	100.45	110.70
3	D	501	N9V	O14-C13-N12	-3.41	116.94	122.29
3	D	501	N9V	O51-P52-O54	-3.31	97.55	109.33
3	A	502	N9V	O14-C13-N12	-3.30	117.11	122.29
2	B	501	NDP	O3-PA-O1A	-3.28	100.83	110.70
2	C	501	NDP	C2B-C1B-N9A	-3.19	108.50	113.75
2	A	501	NDP	N3A-C4A-N9A	3.09	132.42	127.17
3	D	501	N9V	C22-C21-C20	2.96	113.82	108.77
2	A	501	NDP	O3-PA-O1A	-2.96	101.81	110.70
2	D	502	NDP	C2B-C1B-N9A	-2.93	108.93	113.75
3	D	501	N9V	O29-P30-O31	-2.86	102.09	110.70
2	C	501	NDP	N3A-C4A-N9A	2.86	132.04	127.17
3	A	502	N9V	C44-N40-C41	2.78	108.65	105.74
2	A	501	NDP	O2B-P2B-O1X	-2.76	99.49	109.33
3	D	501	N9V	C10-S09-C07	-2.75	93.85	101.73
2	D	502	NDP	N3A-C4A-N9A	2.68	131.72	127.17
2	C	501	NDP	C5A-C4A-N3A	-2.68	123.03	126.72
2	C	501	NDP	C5D-C4D-C3D	-2.66	105.62	115.21
3	D	501	N9V	C23-C21-C24	-2.64	103.87	108.22
2	B	501	NDP	N3A-C4A-N9A	2.61	131.61	127.17
2	D	502	NDP	C5A-C4A-N3A	-2.59	123.16	126.72
2	B	501	NDP	C5A-C4A-N3A	-2.57	123.17	126.72
3	A	502	N9V	O51-P52-O54	-2.56	100.20	109.33
2	D	502	NDP	C3B-C2B-C1B	-2.54	97.95	102.81
2	D	502	NDP	O2N-PN-O3	2.52	114.08	107.27
2	C	501	NDP	O2N-PN-O3	2.47	113.95	107.27
3	D	501	N9V	C44-N40-C41	2.46	108.32	105.74
3	A	502	N9V	C10-S09-C07	2.45	108.77	101.73
2	A	501	NDP	O7N-C7N-N7N	-2.45	117.41	122.89
2	D	502	NDP	O2B-P2B-O1X	-2.42	100.70	109.33
2	C	501	NDP	O7N-C7N-N7N	-2.42	117.47	122.89
2	C	501	NDP	O2B-P2B-O1X	-2.41	100.74	109.33
2	D	502	NDP	C5D-C4D-C3D	-2.41	106.54	115.21
2	B	501	NDP	O2B-P2B-O1X	-2.38	100.86	109.33
3	D	501	N9V	C22-C21-C24	-2.34	104.37	108.22
2	A	501	NDP	O2N-PN-O1N	2.31	123.20	112.44
3	A	502	N9V	O29-P30-O31	-2.24	103.96	110.70
2	C	501	NDP	C3B-C2B-C1B	-2.20	98.59	102.81
3	A	502	N9V	C15-C13-N12	2.19	119.87	115.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NDP	O2N-PN-O1N	2.19	122.61	112.44
3	A	502	N9V	C44-N40-C38	-2.16	121.58	126.63
3	A	502	N9V	O05-C04-O06	2.14	128.93	124.08
3	D	501	N9V	O55-P52-O54	2.12	119.11	110.83
2	D	502	NDP	C5B-C4B-C3B	-2.12	107.58	115.21
2	D	502	NDP	O7N-C7N-N7N	-2.11	118.17	122.89
3	A	502	N9V	C22-C21-C24	-2.09	104.77	108.22
2	C	501	NDP	O3X-P2B-O2X	2.09	115.65	107.80
3	D	501	N9V	O28-P26-O25	-2.07	98.16	107.57
3	A	502	N9V	O06-C04-C03	-2.05	113.34	120.19
2	A	501	NDP	O3X-P2B-O2X	2.03	115.42	107.80
2	B	501	NDP	O2N-PN-O1N	2.03	121.90	112.44
2	A	501	NDP	C5B-C4B-C3B	-2.01	107.96	115.21

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	N9V	C01-C02-C03-C04
3	A	502	N9V	C01-C02-C03-C07
3	A	502	N9V	C03-C07-S09-C10
3	A	502	N9V	C24-O25-P26-O27
3	A	502	N9V	C24-O25-P26-O28
3	A	502	N9V	P26-O29-P30-O33
3	D	501	N9V	C01-C02-C03-C04
3	D	501	N9V	C03-C07-S09-C10
3	D	501	N9V	O08-C07-S09-C10
3	D	501	N9V	C24-O25-P26-O28
3	D	501	N9V	C24-O25-P26-O29
3	A	502	N9V	O14-C13-C15-C16
3	A	502	N9V	N12-C13-C15-C16
2	D	502	NDP	O4D-C1D-N1N-C2N
3	A	502	N9V	O08-C07-S09-C10
2	C	501	NDP	C2B-O2B-P2B-O1X
3	D	501	N9V	C01-C02-C03-C07
3	D	501	N9V	O14-C13-C15-C16
2	A	501	NDP	PN-O3-PA-O5B
3	D	501	N9V	P26-O29-P30-O33
3	D	501	N9V	N12-C13-C15-C16
2	C	501	NDP	O4D-C1D-N1N-C2N
3	A	502	N9V	C22-C21-C24-O25
2	A	501	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
2	B	501	NDP	C2B-O2B-P2B-O1X
3	D	501	N9V	C10-C11-N12-C13
3	A	502	N9V	C20-C21-C24-O25
3	A	502	N9V	C24-O25-P26-O29
3	D	501	N9V	C35-C34-O33-P30
2	C	501	NDP	O4B-C4B-C5B-O5B
2	B	501	NDP	O4D-C1D-N1N-C2N
2	D	502	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	O4D-C1D-N1N-C2N
2	C	501	NDP	C3B-C4B-C5B-O5B
2	C	501	NDP	C2N-C3N-C7N-N7N
3	A	502	N9V	C35-C34-O33-P30
2	B	501	NDP	C2D-C1D-N1N-C2N
2	A	501	NDP	C2D-C1D-N1N-C2N
3	D	501	N9V	P26-O29-P30-O32
2	A	501	NDP	O4B-C4B-C5B-O5B
3	A	502	N9V	C23-C21-C24-O25

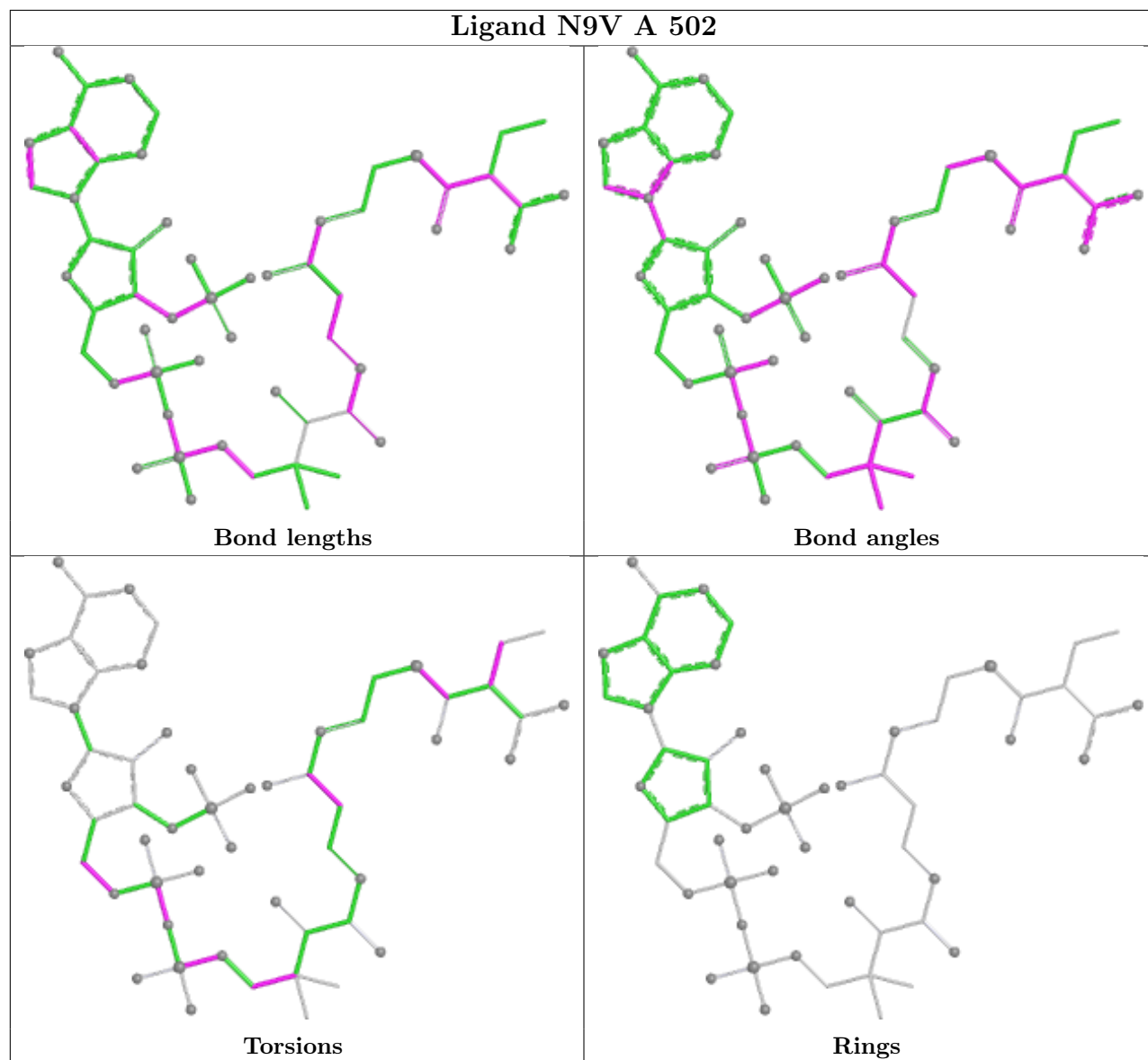
There are no ring outliers.

10 monomers are involved in 21 short contacts:

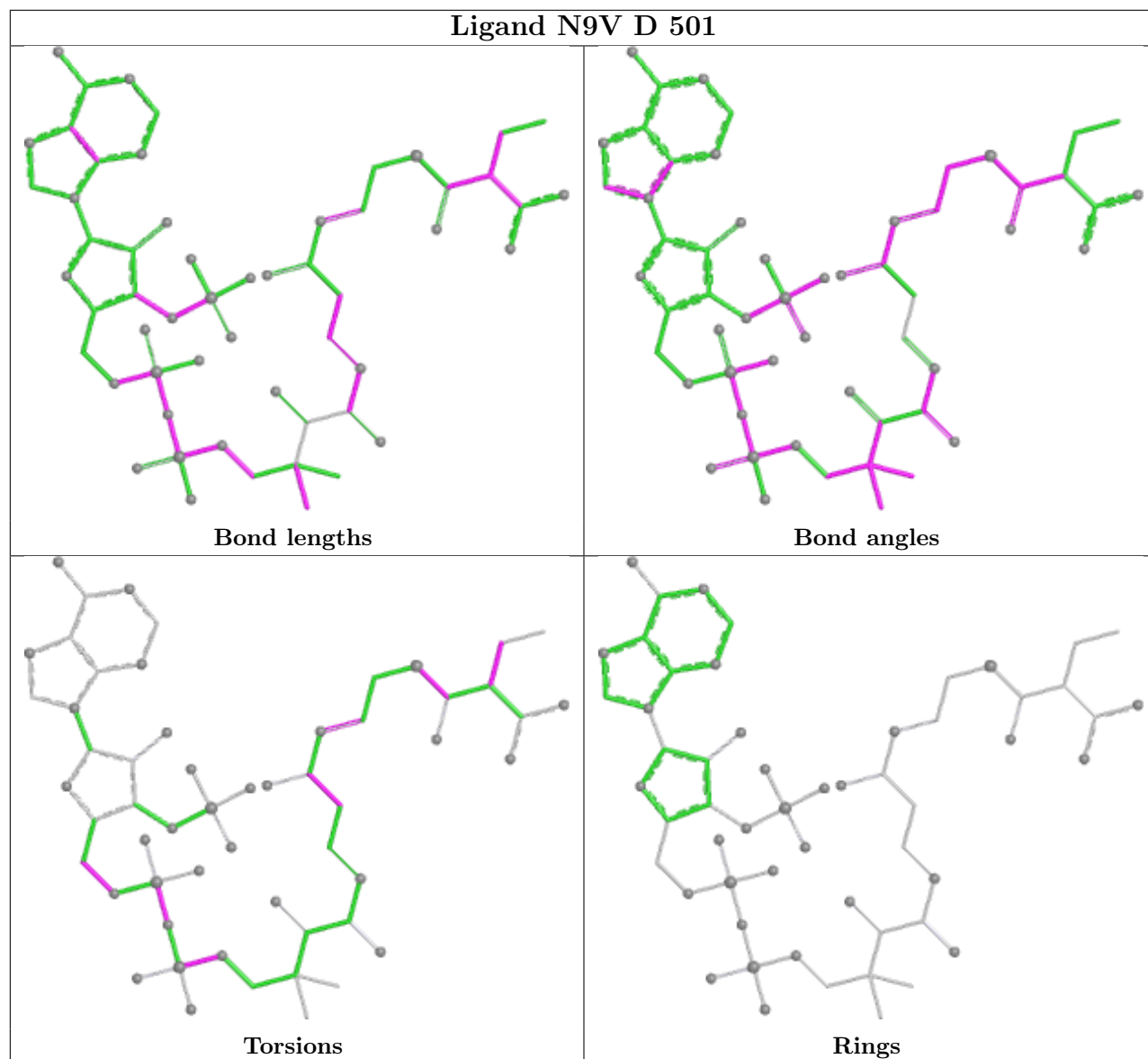
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	IMD	2	0
3	A	502	N9V	5	0
3	D	501	N9V	5	0
4	B	502	IMD	1	0
2	A	501	NDP	2	0
2	C	501	NDP	1	0
4	D	503	IMD	3	0
2	D	502	NDP	2	0
4	A	503	IMD	1	0
2	B	501	NDP	2	0

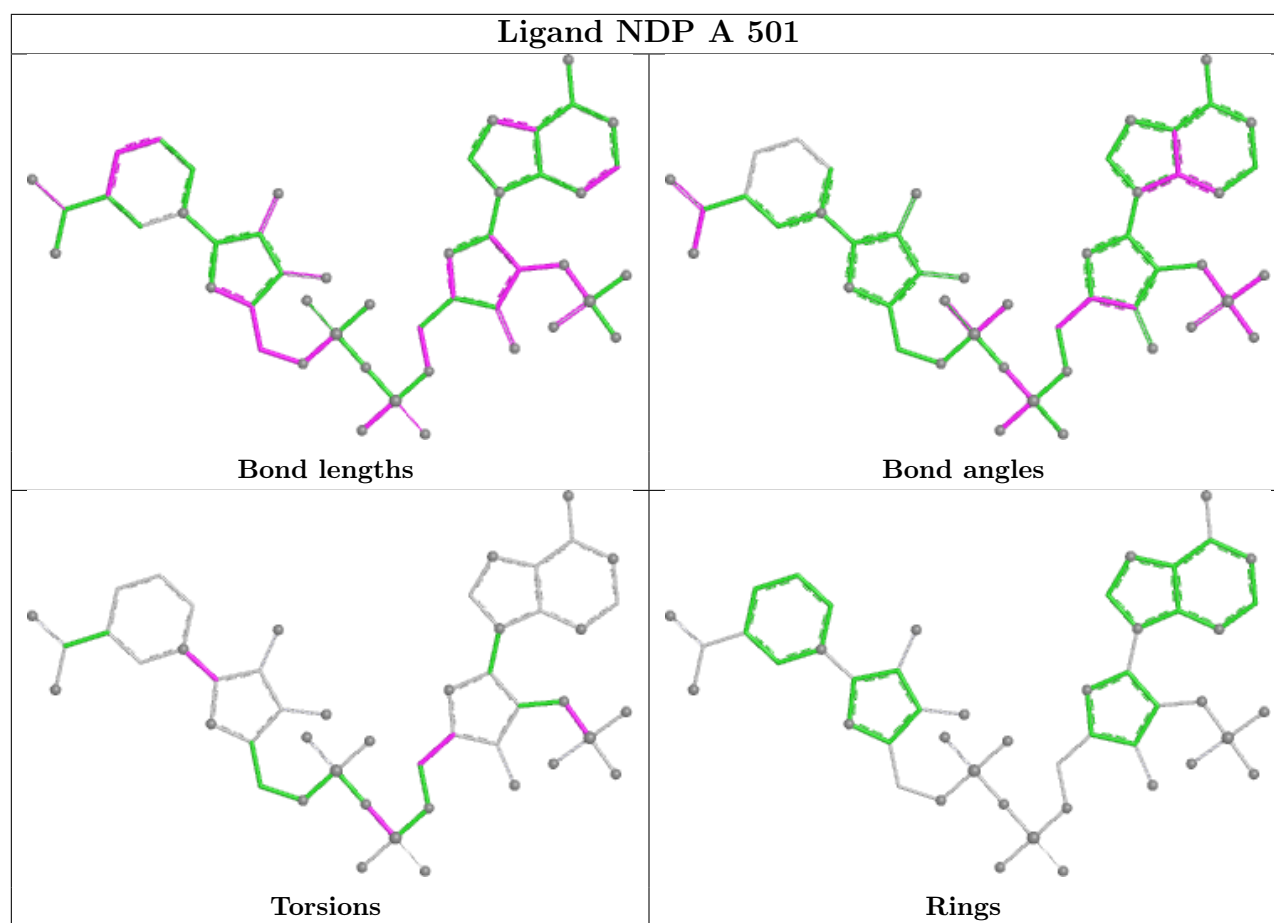
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

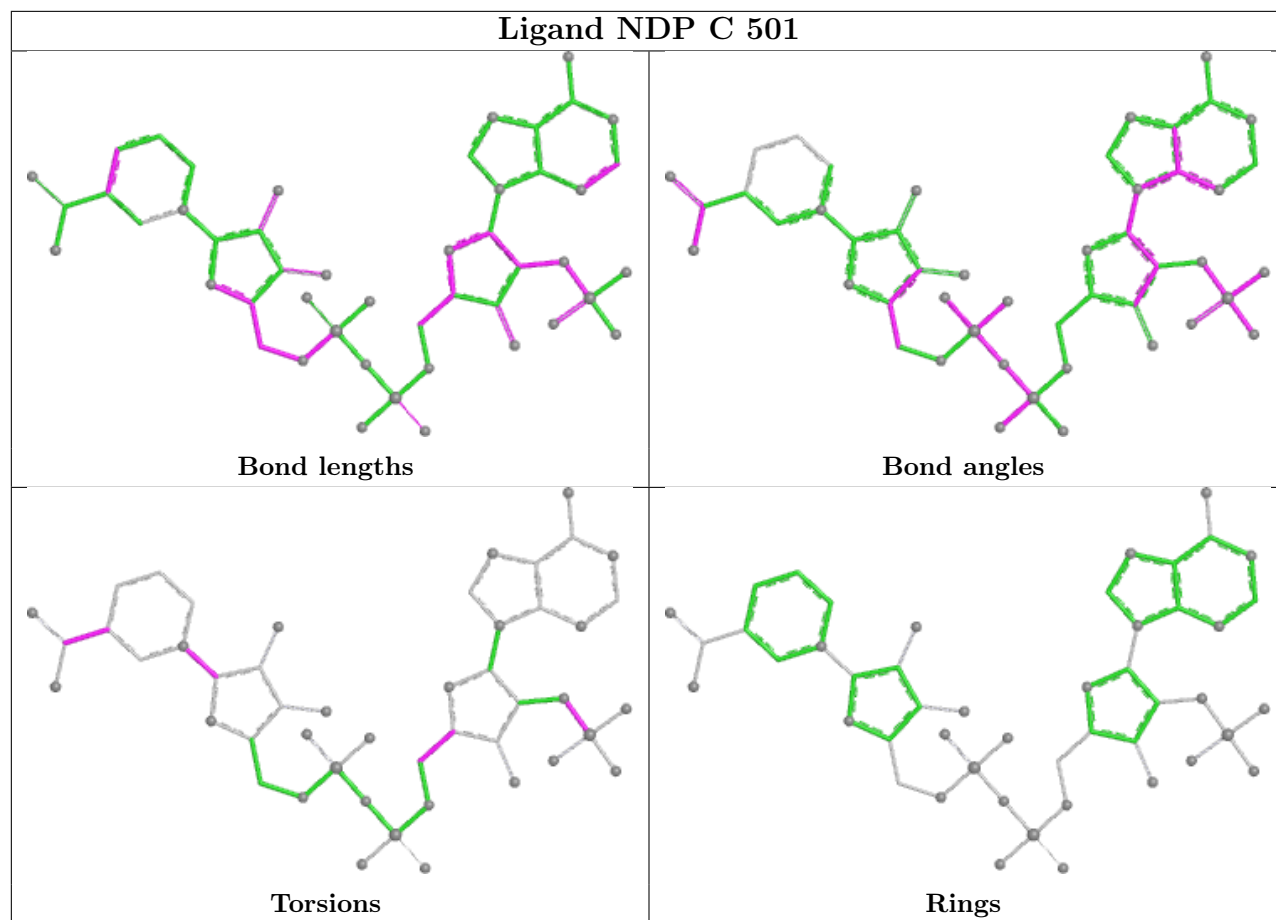
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

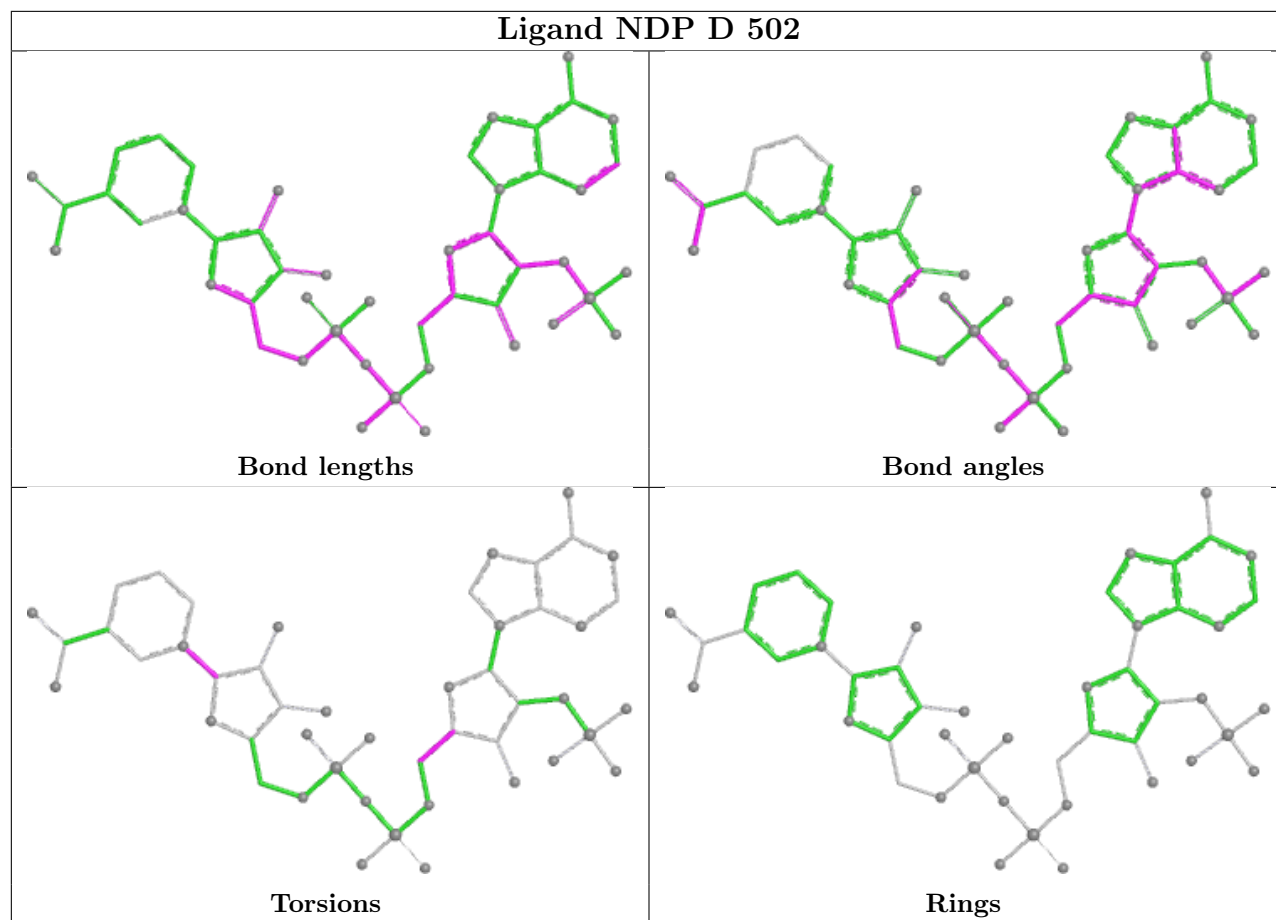


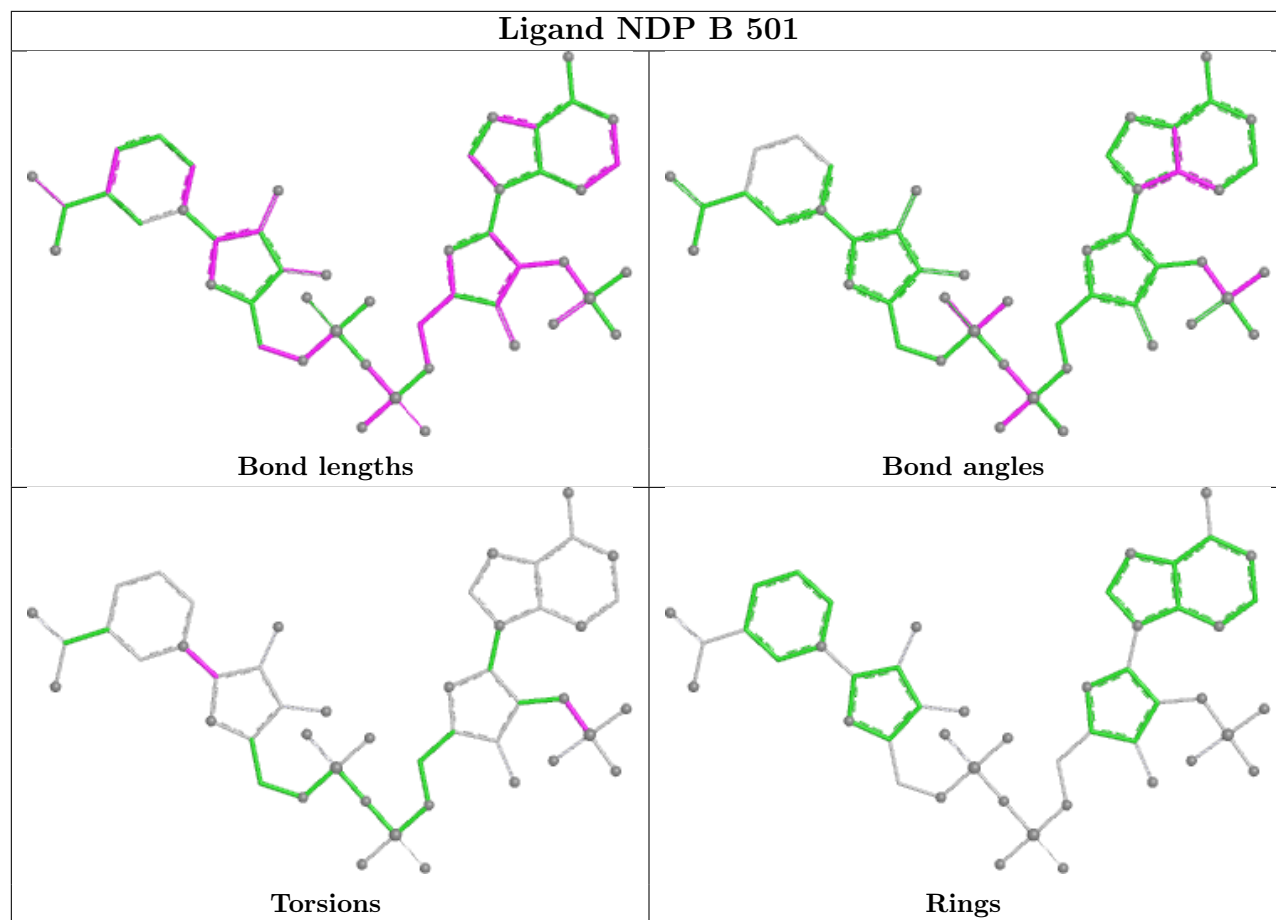
Ligand N9V D 501











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	446/449 (99%)	-0.33	2 (0%) 88 91	7, 22, 40, 67	8 (1%)
1	B	448/449 (99%)	-0.35	1 (0%) 91 93	6, 21, 37, 58	7 (1%)
1	C	447/449 (99%)	-0.27	3 (0%) 84 88	8, 23, 41, 76	7 (1%)
1	D	445/449 (99%)	-0.16	2 (0%) 88 91	8, 24, 43, 59	6 (1%)
All	All	1786/1796 (99%)	-0.28	8 (0%) 88 91	6, 23, 41, 76	28 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	444	ASN	3.8
1	D	134	ALA	2.9
1	A	132	VAL	2.7
1	D	100	TYR	2.4
1	C	42	GLY	2.1
1	A	-1	ARG	2.1
1	B	296[A]	LYS	2.1
1	C	134	ALA	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](#)

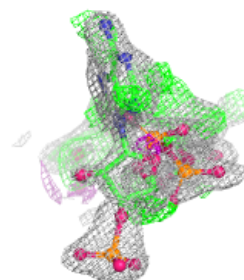
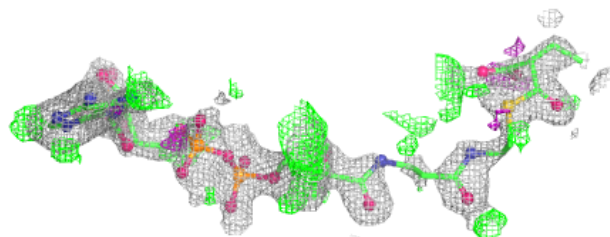
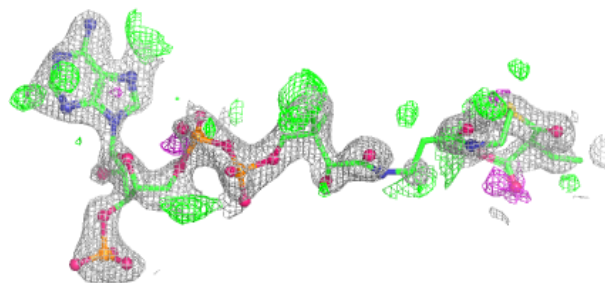
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	N9V	A	502	56/56	0.76	0.17	24,48,75,75	56
3	N9V	D	501	56/56	0.77	0.17	27,44,70,72	56
4	IMD	D	503	5/5	0.80	0.19	46,49,49,50	0
4	IMD	C	502	5/5	0.88	0.14	45,47,48,49	0
4	IMD	A	503	5/5	0.94	0.08	34,36,38,39	0
4	IMD	B	502	5/5	0.94	0.10	33,34,36,37	0
2	NDP	C	501	48/48	0.96	0.08	19,27,46,55	0
2	NDP	D	502	48/48	0.96	0.08	20,27,42,50	0
2	NDP	A	501	48/48	0.98	0.05	16,19,24,25	0
2	NDP	B	501	48/48	0.98	0.05	16,20,24,28	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.

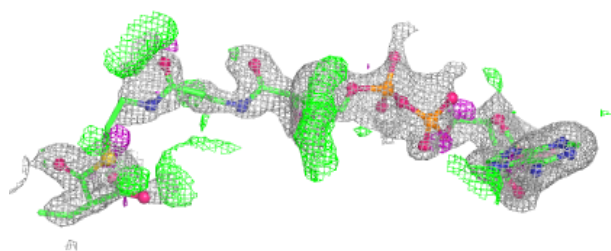
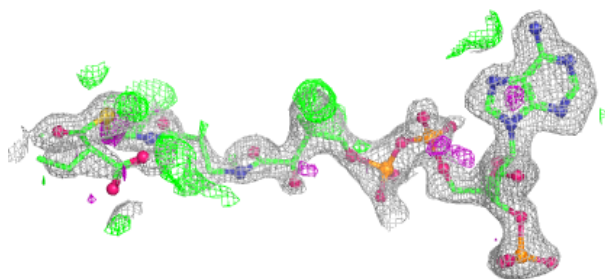
Electron density around N9V A 502:

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

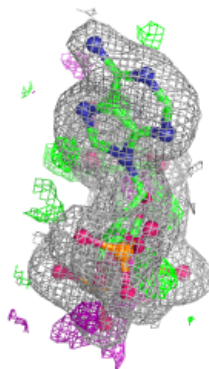
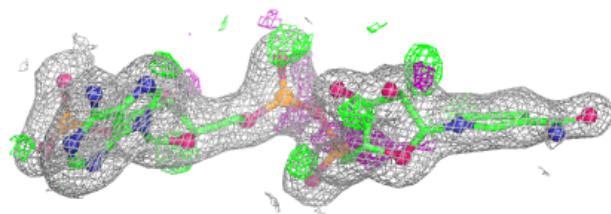
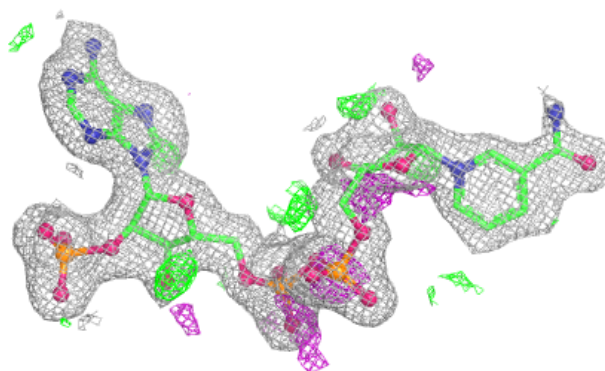


Electron density around N9V D 501:

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

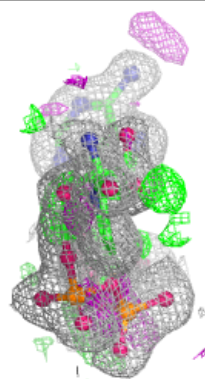
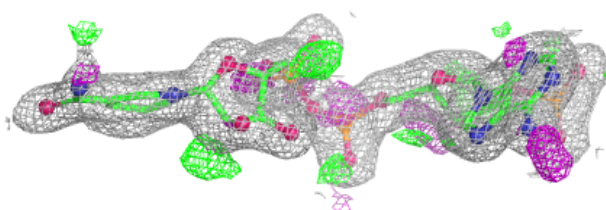
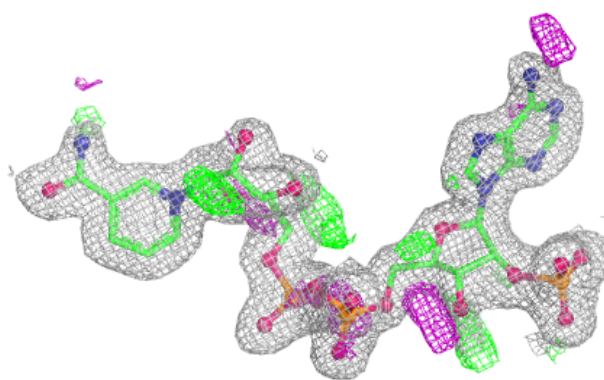
**Electron density around NDP C 501:**

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

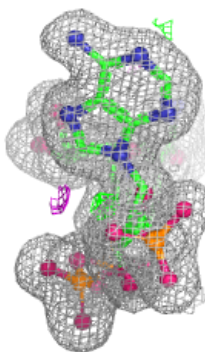
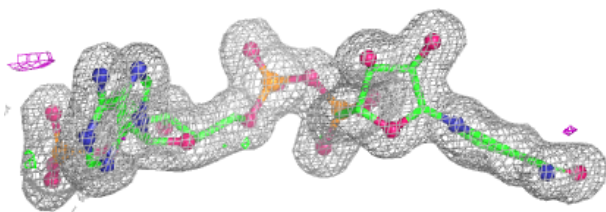
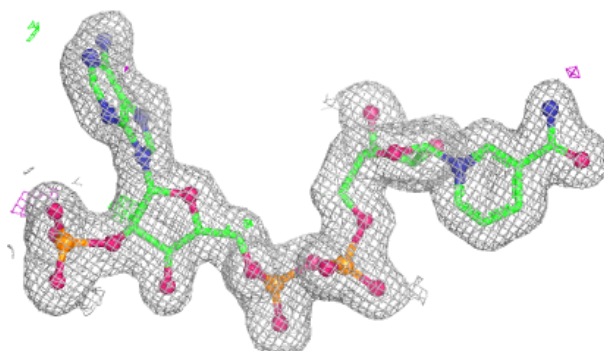


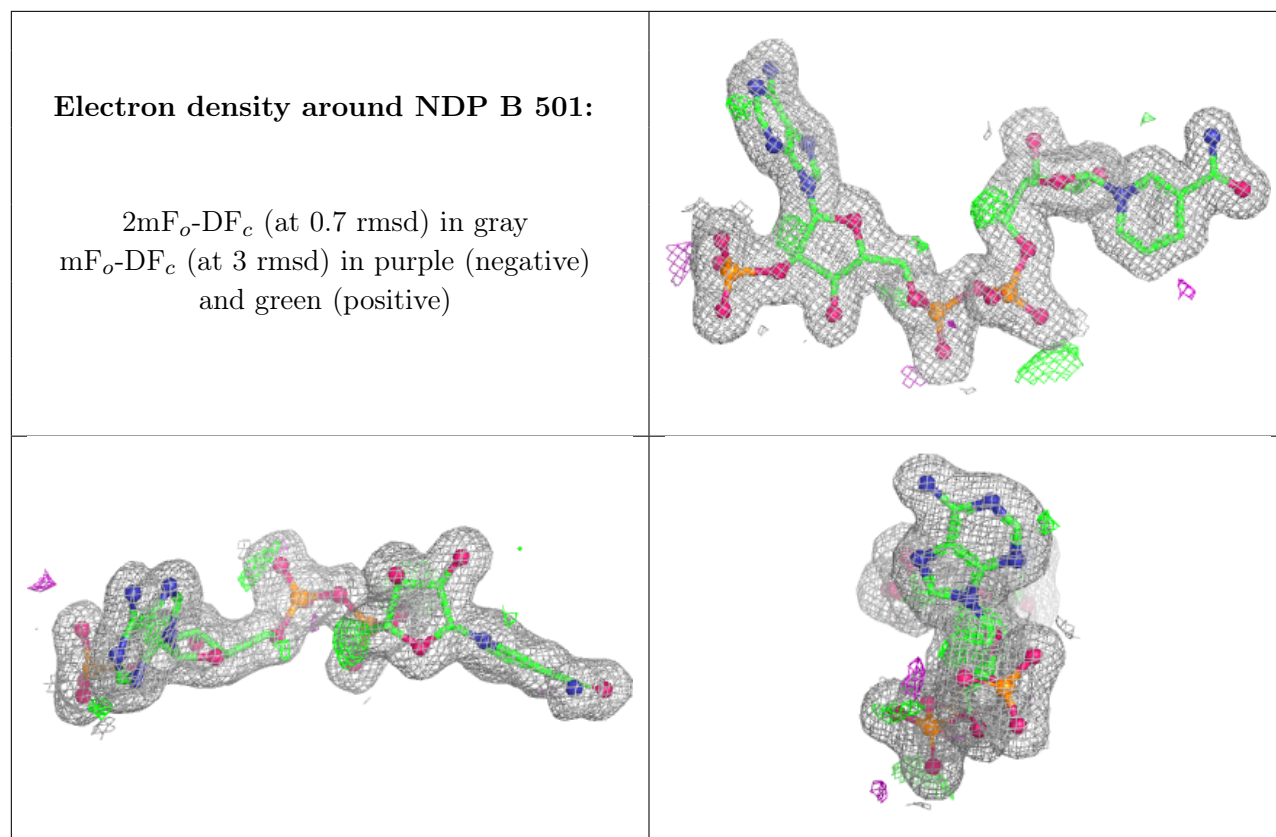
Electron density around NDP D 502:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.