



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:00 pm BST

PDB ID : 3OID
Title : Crystal Structure of Enoyl-ACP Reductases III (FabL) from *B. subtilis* (complex with NADP and TCL)
Authors : Kim, K.-H.; Ha, B.H.; Kim, S.J.; Hong, S.K.; Hwang, K.Y.; Kim, E.E.
Deposited on : 2010-08-19
Resolution : 1.80 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 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

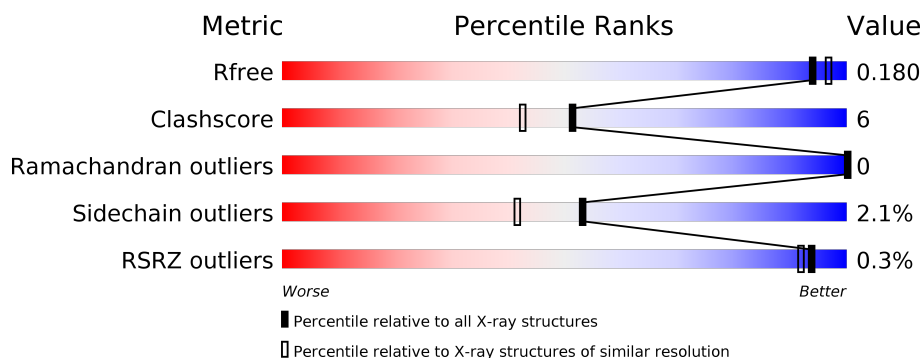
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 ≥ 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	258	<div> <div>86%</div> <div>8%</div> <div>• •</div> </div>
1	B	258	<div> <div>%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	C	258	<div> <div>88%</div> <div>7%</div> <div>• •</div> </div>
1	D	258	<div> <div>87%</div> <div>7%</div> <div>• •</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8384 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 [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1895	1192	332	362	9			
1	B	251	Total	C	N	O	S	0	0	0
			1912	1202	334	366	10			
1	C	248	Total	C	N	O	S	0	0	0
			1886	1187	330	360	9			
1	D	248	Total	C	N	O	S	0	0	0
			1886	1187	330	360	9			

There are 32 discrepancies between the modelled and reference sequences:

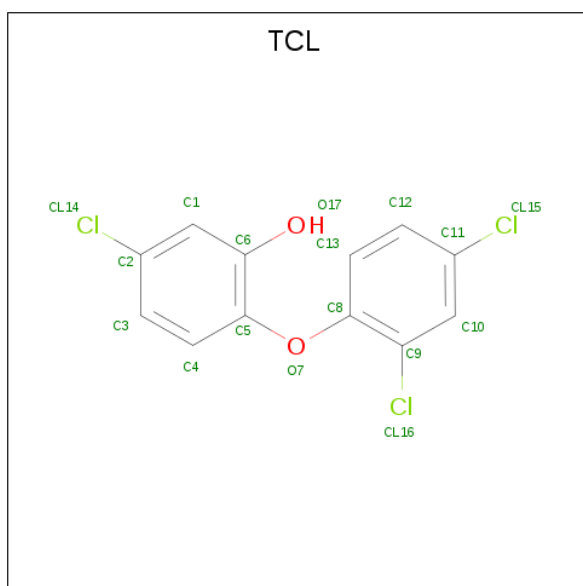
Chain	Residue	Modelled	Actual	Comment	Reference
A	251	LEU	-	EXPRESSION TAG	UNP P71079
A	252	GLU	-	EXPRESSION TAG	UNP P71079
A	253	HIS	-	EXPRESSION TAG	UNP P71079
A	254	HIS	-	EXPRESSION TAG	UNP P71079
A	255	HIS	-	EXPRESSION TAG	UNP P71079
A	256	HIS	-	EXPRESSION TAG	UNP P71079
A	257	HIS	-	EXPRESSION TAG	UNP P71079
A	258	HIS	-	EXPRESSION TAG	UNP P71079
B	251	LEU	-	EXPRESSION TAG	UNP P71079
B	252	GLU	-	EXPRESSION TAG	UNP P71079
B	253	HIS	-	EXPRESSION TAG	UNP P71079
B	254	HIS	-	EXPRESSION TAG	UNP P71079
B	255	HIS	-	EXPRESSION TAG	UNP P71079
B	256	HIS	-	EXPRESSION TAG	UNP P71079
B	257	HIS	-	EXPRESSION TAG	UNP P71079
B	258	HIS	-	EXPRESSION TAG	UNP P71079
C	251	LEU	-	EXPRESSION TAG	UNP P71079
C	252	GLU	-	EXPRESSION TAG	UNP P71079
C	253	HIS	-	EXPRESSION TAG	UNP P71079
C	254	HIS	-	EXPRESSION TAG	UNP P71079
C	255	HIS	-	EXPRESSION TAG	UNP P71079

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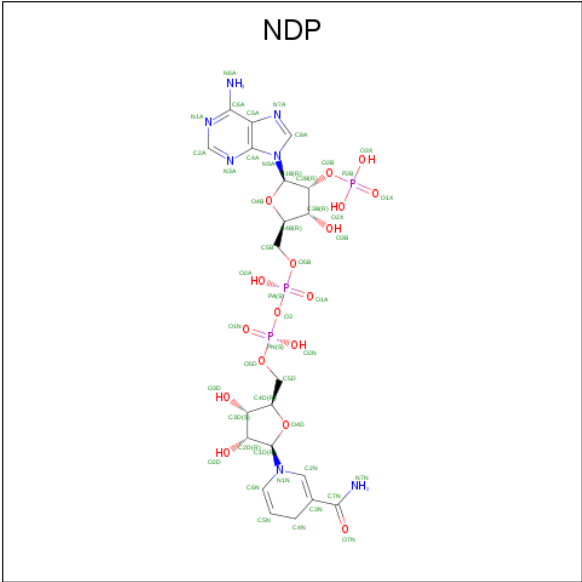
Chain	Residue	Modelled	Actual	Comment	Reference
C	256	HIS	-	EXPRESSION TAG	UNP P71079
C	257	HIS	-	EXPRESSION TAG	UNP P71079
C	258	HIS	-	EXPRESSION TAG	UNP P71079
D	251	LEU	-	EXPRESSION TAG	UNP P71079
D	252	GLU	-	EXPRESSION TAG	UNP P71079
D	253	HIS	-	EXPRESSION TAG	UNP P71079
D	254	HIS	-	EXPRESSION TAG	UNP P71079
D	255	HIS	-	EXPRESSION TAG	UNP P71079
D	256	HIS	-	EXPRESSION TAG	UNP P71079
D	257	HIS	-	EXPRESSION TAG	UNP P71079
D	258	HIS	-	EXPRESSION TAG	UNP P71079

- Molecule 2 is TRICLOSAN (three-letter code: TCL) (formula: C₁₂H₇Cl₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	D	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	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		
3	D	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	138	Total	O	0	0
			138	138		
4	B	134	Total	O	0	0
			134	134		
4	C	139	Total	O	0	0
			139	139		
4	D	134	Total	O	0	0
			134	134		

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.

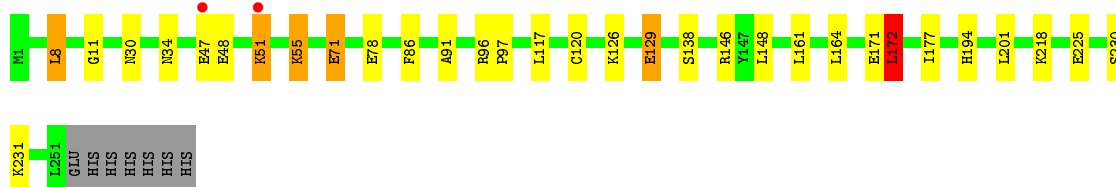
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

Chain A:  86% 8% . .




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

Chain B:  85% 10% . .



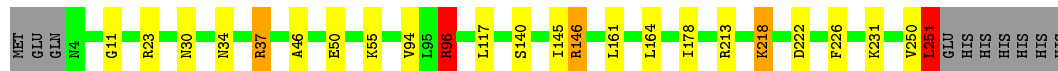
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADPH]

Chain C:  88% 7% . .



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

Chain D:  87% 7% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.38Å 110.68Å 85.17Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	36.01 – 1.80 36.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.01-1.80) 99.1 (36.01-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.48 (at 1.79Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0109	Depositor
R, R_{free}	0.149 , 0.181 0.148 , 0.180	Depositor DCC
R_{free} test set	4970 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8384	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.26	4/1917 (0.2%)	1.04	6/2588 (0.2%)
1	B	1.23	5/1934 (0.3%)	1.02	5/2610 (0.2%)
1	C	1.22	3/1908 (0.2%)	1.04	6/2576 (0.2%)
1	D	1.23	1/1908 (0.1%)	1.07	11/2576 (0.4%)
All	All	1.24	13/7667 (0.2%)	1.04	28/10350 (0.3%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	GLU	CG-CD	8.04	1.64	1.51
1	A	225	GLU	CD-OE1	-7.90	1.17	1.25
1	C	203	GLU	CG-CD	6.99	1.62	1.51
1	B	225	GLU	CD-OE1	-6.06	1.19	1.25
1	B	78	GLU	CG-CD	5.83	1.60	1.51
1	C	73	PHE	CE2-CZ	5.71	1.48	1.37
1	A	6	CYS	CB-SG	5.63	1.91	1.82
1	B	91	ALA	CA-CB	5.51	1.64	1.52
1	D	226	PHE	CD2-CE2	5.36	1.50	1.39
1	C	211	ALA	CA-CB	5.23	1.63	1.52
1	A	199	GLU	CB-CG	5.14	1.61	1.52
1	B	129	GLU	CG-CD	5.09	1.59	1.51
1	B	71	GLU	CB-CG	5.08	1.61	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	D	146	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	C	146	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	40	LYS	CD-CE-NZ	-8.17	92.91	111.70
1	D	37	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	146	ARG	NE-CZ-NH1	-7.53	116.53	120.30
1	D	213	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	146	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	8	LEU	CB-CG-CD2	6.77	122.51	111.00
1	D	251	LEU	CB-CG-CD1	-6.65	99.70	111.00
1	D	96	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	98	VAL	CG1-CB-CG2	-6.56	100.40	110.90
1	D	251	LEU	CA-CB-CG	6.46	130.15	115.30
1	D	178	ILE	CG1-CB-CG2	-6.36	97.41	111.40
1	D	251	LEU	CB-CG-CD2	6.18	121.50	111.00
1	B	172	LEU	CB-CG-CD1	6.18	121.50	111.00
1	A	250	VAL	C-N-CA	6.06	136.85	121.70
1	A	166	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	8	LEU	CB-CG-CD1	5.73	120.74	111.00
1	D	164	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	B	55	LYS	CD-CE-NZ	-5.55	98.94	111.70
1	C	146	ARG	CG-CD-NE	-5.52	100.21	111.80
1	D	146	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	D	222	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	251	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	B	201	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	C	250	VAL	C-N-CA	5.23	134.78	121.70
1	B	164	LEU	CB-CG-CD2	-5.09	102.35	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	LEU	Peptide

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1895	0	1948	22	0
1	B	1912	0	1966	28	0
1	C	1886	0	1940	16	0
1	D	1886	0	1940	24	0
2	A	17	0	6	0	0
2	B	17	0	6	0	0
2	C	17	0	6	0	0
2	D	17	0	6	0	0
3	A	48	0	26	2	0
3	B	48	0	26	1	0
3	C	48	0	26	2	0
3	D	48	0	26	3	0
4	A	138	0	0	5	0
4	B	134	0	0	9	0
4	C	139	0	0	3	0
4	D	134	0	0	1	0
All	All	8384	0	7922	88	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 6.

All (88) 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:B:218:LYS:HE3	4:B:296:HOH:O	1.40	1.21
1:B:71:GLU:HG3	4:B:364:HOH:O	1.36	1.20
1:D:23:ARG:NH2	1:D:218:LYS:HD2	1.71	1.05
1:D:23:ARG:NH2	1:D:218:LYS:CD	2.29	0.95
4:A:323:HOH:O	1:C:251:LEU:HB3	1.75	0.84
1:D:23:ARG:HH21	1:D:218:LYS:CD	1.91	0.82
1:C:11:GLY:H	1:C:34:ASN:HD22	1.30	0.80
1:C:4:ASN:N	4:C:294:HOH:O	2.15	0.79
1:B:71:GLU:CG	4:B:364:HOH:O	2.08	0.78
1:A:199:GLU:CD	1:A:199:GLU:H	1.88	0.77
1:B:8:LEU:HD12	1:B:86:PHE:CD1	2.23	0.73
1:A:11:GLY:H	1:A:34:ASN:HD22	1.37	0.72
1:B:11:GLY:H	1:B:34:ASN:HD22	1.37	0.70
1:D:11:GLY:H	1:D:34:ASN:HD22	1.40	0.69
1:B:8:LEU:HD12	1:B:86:PHE:HD1	1.56	0.69
1:A:94:VAL:HG12	1:A:96:ARG:HD3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:HIS:HE1	4:B:446:HOH:O	1.78	0.67
1:D:23:ARG:HH22	1:D:218:LYS:HD2	1.58	0.66
1:B:129:GLU:HB3	4:B:336:HOH:O	1.97	0.65
1:D:23:ARG:HH21	1:D:218:LYS:HD2	1.51	0.63
1:A:30:ASN:HD22	1:A:55:LYS:H	1.45	0.63
1:B:30:ASN:HD22	1:B:55:LYS:H	1.46	0.61
1:C:251:LEU:HD12	1:C:251:LEU:N	2.14	0.61
1:B:48:GLU:OE2	4:B:312:HOH:O	2.16	0.60
1:C:230:SER:N	4:C:465:HOH:O	2.22	0.60
1:A:230:SER:N	4:A:449:HOH:O	2.31	0.60
1:D:23:ARG:NH2	1:D:218:LYS:HD3	2.17	0.59
1:B:8:LEU:C	1:B:8:LEU:HD13	2.21	0.59
1:D:23:ARG:HH22	1:D:218:LYS:CD	2.10	0.58
1:B:138:SER:HB3	1:B:161:LEU:HD11	1.85	0.58
1:A:194:HIS:HE1	4:A:316:HOH:O	1.86	0.58
1:A:231:LYS:HE2	4:B:451:HOH:O	2.04	0.58
1:D:23:ARG:HH21	1:D:218:LYS:CE	2.17	0.57
1:A:94:VAL:CG1	1:A:96:ARG:HD3	2.35	0.56
1:B:11:GLY:HA2	3:B:503:NDP:H1B	1.88	0.56
1:B:117:LEU:HD22	1:B:161:LEU:HD22	1.88	0.55
1:D:30:ASN:ND2	1:D:55:LYS:H	2.05	0.54
1:C:229:SER:O	1:C:230:SER:CB	2.56	0.54
1:B:171:GLU:OE1	1:C:98:VAL:HG23	2.07	0.54
1:D:117:LEU:HD22	1:D:161:LEU:HD22	1.90	0.53
1:A:96:ARG:HB2	1:A:97:PRO:CD	2.39	0.53
1:B:48:GLU:O	1:B:51:LYS:HG2	2.09	0.52
1:A:192:LEU:HB3	1:A:198:ARG:HG3	1.91	0.52
1:C:161:LEU:C	1:C:161:LEU:HD23	2.30	0.52
1:A:30:ASN:ND2	1:A:55:LYS:H	2.08	0.52
1:B:30:ASN:ND2	1:B:55:LYS:H	2.08	0.51
1:C:131:ASN:HB2	4:C:534:HOH:O	2.10	0.51
4:B:463:HOH:O	1:D:251:LEU:HD22	2.12	0.50
1:C:190:ASP:O	1:C:193:LYS:HG2	2.13	0.49
1:C:30:ASN:ND2	1:C:55:LYS:H	2.11	0.49
4:A:348:HOH:O	1:B:231:LYS:HE2	2.12	0.49
1:C:140:SER:O	3:C:504:NDP:H6N	2.12	0.48
1:D:117:LEU:CD2	1:D:161:LEU:HD22	2.43	0.48
1:D:11:GLY:HA2	3:D:502:NDP:H1B	1.93	0.48
1:D:140:SER:O	3:D:502:NDP:H6N	2.12	0.48
1:B:126:LYS:O	1:B:129:GLU:HG2	2.13	0.48
1:A:143:GLY:HA2	1:A:148:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:VAL:HG12	1:A:251:LEU:N	2.29	0.47
1:A:197:ASN:OD1	4:A:493:HOH:O	2.21	0.47
1:D:146:ARG:NH2	4:D:315:HOH:O	2.32	0.47
1:B:230:SER:N	4:B:349:HOH:O	2.40	0.46
1:B:11:GLY:H	1:B:34:ASN:ND2	2.10	0.46
1:B:138:SER:CB	1:B:161:LEU:HD11	2.46	0.45
1:B:96:ARG:HB2	1:B:97:PRO:CD	2.47	0.45
1:B:148:LEU:HD13	1:D:250:VAL:HG13	1.97	0.45
1:C:229:SER:O	1:C:230:SER:HB2	2.16	0.45
1:C:11:GLY:HA2	3:C:504:NDP:H1B	1.98	0.45
1:B:96:ARG:HB2	1:B:97:PRO:HD2	1.99	0.45
1:D:30:ASN:HD22	1:D:55:LYS:H	1.63	0.45
1:A:145:ILE:HG13	1:A:146:ARG:HG2	1.98	0.44
1:D:34:ASN:HD21	3:D:502:NDP:H2A	1.81	0.44
1:A:140:SER:O	3:A:501:NDP:H6N	2.17	0.44
1:A:96:ARG:HB2	1:A:97:PRO:HD2	1.99	0.43
1:C:35:TYR:CZ	1:C:60:LYS:HB2	2.54	0.42
1:A:11:GLY:HA2	3:A:501:NDP:H1B	2.01	0.42
1:D:94:VAL:CG1	1:D:96:ARG:HD3	2.50	0.42
1:B:172:LEU:HB3	1:B:177:ILE:HB	2.01	0.42
1:A:193:LYS:HD2	1:A:198:ARG:CD	2.50	0.42
1:D:117:LEU:HD22	1:D:161:LEU:CD2	2.49	0.42
1:D:94:VAL:HG12	1:D:96:ARG:HD3	2.02	0.42
1:B:117:LEU:CD2	1:B:161:LEU:HD22	2.50	0.41
1:B:86:PHE:CZ	1:B:120:CYS:HB3	2.55	0.41
1:C:11:GLY:H	1:C:34:ASN:ND2	2.07	0.41
1:A:193:LYS:HD2	1:A:198:ARG:HD3	2.01	0.41
1:D:46:ALA:O	1:D:50:GLU:HG3	2.21	0.41
1:A:251:LEU:HA	1:A:251:LEU:HD22	1.24	0.40
1:A:250:VAL:C	1:A:251:LEU:HD23	2.42	0.40
1:D:145:ILE:HG13	1:D:146:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/258 (96%)	240 (97%)	7 (3%)	0	100	100
1	B	249/258 (96%)	245 (98%)	4 (2%)	0	100	100
1	C	246/258 (95%)	242 (98%)	4 (2%)	0	100	100
1	D	246/258 (95%)	241 (98%)	5 (2%)	0	100	100
All	All	988/1032 (96%)	968 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/211 (96%)	197 (98%)	5 (2%)	47	34
1	B	204/211 (97%)	200 (98%)	4 (2%)	55	44
1	C	201/211 (95%)	198 (98%)	3 (2%)	65	56
1	D	201/211 (95%)	196 (98%)	5 (2%)	47	34
All	All	808/844 (96%)	791 (98%)	17 (2%)	53	42

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	96	ARG
1	A	199	GLU
1	A	231	LYS
1	A	251	LEU
1	B	8	LEU
1	B	47	GLU
1	B	51	LYS
1	B	172	LEU
1	C	98	VAL

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Mol	Chain	Res	Type
1	C	193	LYS
1	C	230	SER
1	D	37	ARG
1	D	96	ARG
1	D	218	LYS
1	D	231	LYS
1	D	251	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	34	ASN
1	A	65	GLN
1	A	194	HIS
1	B	4	ASN
1	B	30	ASN
1	B	34	ASN
1	B	131	ASN
1	B	194	HIS
1	C	30	ASN
1	C	34	ASN
1	C	74	GLN
1	D	30	ASN
1	D	34	ASN

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	C	504	-	45,52,52	1.57	4 (8%)	53,80,80	1.47	10 (18%)
2	TCL	D	602	-	18,18,18	1.58	4 (22%)	25,25,25	1.63	3 (12%)
3	NDP	B	503	-	45,52,52	1.57	7 (15%)	53,80,80	1.47	6 (11%)
3	NDP	A	501	-	45,52,52	1.34	3 (6%)	53,80,80	1.73	8 (15%)
3	NDP	D	502	-	45,52,52	1.30	3 (6%)	53,80,80	1.58	8 (15%)
2	TCL	B	603	-	18,18,18	1.61	2 (11%)	25,25,25	2.11	7 (28%)
2	TCL	C	604	-	18,18,18	1.54	2 (11%)	25,25,25	1.52	5 (20%)
2	TCL	A	601	-	18,18,18	1.65	3 (16%)	25,25,25	2.23	9 (36%)

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	C	504	-	-	6/30/77/77	0/5/5/5
2	TCL	D	602	-	-	0/4/4/4	0/2/2/2
3	NDP	B	503	-	-	6/30/77/77	0/5/5/5
3	NDP	A	501	-	-	5/30/77/77	0/5/5/5
3	NDP	D	502	-	-	6/30/77/77	0/5/5/5
2	TCL	B	603	-	-	0/4/4/4	0/2/2/2
2	TCL	C	604	-	-	0/4/4/4	0/2/2/2
2	TCL	A	601	-	-	0/4/4/4	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	504	NDP	O7N-C7N	5.62	1.37	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	504	NDP	C2A-N3A	4.93	1.40	1.32
3	A	501	NDP	O7N-C7N	4.73	1.35	1.24
3	B	503	NDP	O7N-C7N	4.41	1.34	1.24
2	C	604	TCL	C6-C5	4.18	1.47	1.40
3	A	501	NDP	C2A-N3A	4.12	1.38	1.32
3	D	502	NDP	O7N-C7N	4.04	1.34	1.24
2	A	601	TCL	C6-C5	3.94	1.47	1.40
3	B	503	NDP	C2A-N3A	3.88	1.38	1.32
2	B	603	TCL	C6-C5	3.86	1.47	1.40
2	A	601	TCL	C8-C9	3.80	1.46	1.39
2	D	602	TCL	C6-C5	3.77	1.47	1.40
2	D	602	TCL	C8-C9	3.63	1.46	1.39
3	B	503	NDP	C6N-C5N	3.60	1.39	1.33
3	C	504	NDP	O4B-C1B	3.56	1.46	1.41
3	D	502	NDP	C2A-N3A	3.38	1.37	1.32
3	B	503	NDP	O4B-C1B	3.08	1.45	1.41
3	C	504	NDP	C6N-C5N	3.01	1.38	1.33
2	C	604	TCL	C8-C9	3.01	1.44	1.39
3	B	503	NDP	P2B-O2B	2.96	1.64	1.59
2	B	603	TCL	C8-C9	2.71	1.44	1.39
3	A	501	NDP	O4B-C1B	2.57	1.44	1.41
3	B	503	NDP	PA-O2A	-2.51	1.43	1.55
3	D	502	NDP	P2B-O2B	2.41	1.63	1.59
2	D	602	TCL	O7-C8	-2.22	1.34	1.39
2	A	601	TCL	C11-CL15	2.18	1.79	1.74
2	D	602	TCL	C9-CL16	2.16	1.78	1.73
3	B	503	NDP	O3D-C3D	2.01	1.47	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NDP	N3A-C2A-N1A	-6.60	118.36	128.68
2	A	601	TCL	C9-C10-C11	-6.21	111.77	118.71
3	D	502	NDP	N3A-C2A-N1A	-5.77	119.65	128.68
3	B	503	NDP	O7N-C7N-C3N	-4.92	111.63	120.90
3	D	502	NDP	C3N-C7N-N7N	4.75	126.10	117.67
3	A	501	NDP	C5A-C6A-N6A	4.68	127.47	120.35
2	D	602	TCL	C10-C11-CL15	-4.64	113.35	119.15
2	B	603	TCL	C12-C11-C10	4.64	127.69	121.53
2	B	603	TCL	C10-C11-CL15	-4.50	113.53	119.15
3	C	504	NDP	O7N-C7N-C3N	-4.35	112.71	120.90
2	B	603	TCL	C9-C10-C11	-4.28	113.93	118.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	NDP	C3N-C2N-N1N	-4.25	117.03	123.10
2	A	601	TCL	C12-C11-C10	4.08	126.94	121.53
2	D	602	TCL	C12-C11-C10	3.93	126.76	121.53
3	A	501	NDP	C2A-N1A-C6A	3.77	125.21	118.75
2	B	603	TCL	C1-C2-CL14	-3.68	114.55	119.15
2	C	604	TCL	C9-C10-C11	-3.67	114.61	118.71
2	A	601	TCL	C10-C11-CL15	-3.66	114.58	119.15
3	B	503	NDP	N3A-C2A-N1A	-3.54	123.14	128.68
2	A	601	TCL	C1-C2-CL14	-3.50	114.77	119.15
3	B	503	NDP	C3N-C7N-N7N	3.45	123.80	117.67
3	C	504	NDP	C3N-C2N-N1N	-3.45	118.18	123.10
3	D	502	NDP	O7N-C7N-C3N	-3.35	114.58	120.90
3	C	504	NDP	C3N-C7N-N7N	3.31	123.55	117.67
3	A	501	NDP	C1D-N1N-C6N	-3.28	113.77	120.83
2	D	602	TCL	C9-C10-C11	-3.24	115.09	118.71
3	A	501	NDP	O7N-C7N-C3N	-3.19	114.89	120.90
3	A	501	NDP	C3N-C2N-N1N	-2.93	118.92	123.10
3	D	502	NDP	C2A-N1A-C6A	2.90	123.71	118.75
2	A	601	TCL	C12-C13-C8	-2.66	114.99	120.06
2	C	604	TCL	C12-C11-C10	2.64	125.03	121.53
3	C	504	NDP	O3D-C3D-C2D	-2.59	103.44	111.82
2	A	601	TCL	C3-C2-C1	2.58	124.96	121.53
2	C	604	TCL	C10-C11-CL15	-2.57	115.94	119.15
3	C	504	NDP	N3A-C2A-N1A	-2.57	124.66	128.68
3	D	502	NDP	C5A-C6A-N6A	2.51	124.16	120.35
2	A	601	TCL	C10-C9-C8	2.40	124.23	121.02
2	A	601	TCL	C6-C1-C2	-2.35	116.16	118.98
3	C	504	NDP	O4B-C1B-C2B	-2.34	102.52	106.59
2	B	603	TCL	C6-C1-C2	-2.33	116.19	118.98
3	B	503	NDP	C1D-N1N-C6N	-2.31	115.86	120.83
2	B	603	TCL	C12-C13-C8	-2.29	115.69	120.06
3	D	502	NDP	C1D-N1N-C6N	-2.26	115.95	120.83
3	C	504	NDP	O2A-PA-O1A	2.26	123.42	112.24
3	C	504	NDP	C4A-C5A-N7A	-2.24	107.06	109.40
3	C	504	NDP	O4D-C1D-C2D	-2.24	101.75	106.64
2	A	601	TCL	C8-C9-CL16	-2.21	116.83	119.43
2	C	604	TCL	C3-C2-C1	2.19	124.44	121.53
3	A	501	NDP	C3B-C2B-C1B	-2.18	98.80	102.89
2	B	603	TCL	C13-C8-C9	2.15	122.23	118.84
3	C	504	NDP	C1D-N1N-C6N	-2.14	116.22	120.83
3	B	503	NDP	O4B-C1B-C2B	-2.10	102.94	106.59
3	D	502	NDP	C5B-C4B-C3B	-2.10	107.32	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NDP	O2N-PN-O1N	2.05	122.37	112.24
3	D	502	NDP	O3B-C3B-C2B	-2.02	105.44	111.17
2	C	604	TCL	C8-C9-CL16	-2.00	117.08	119.43

There are no chirality outliers.

All (23) torsion outliers are listed below:

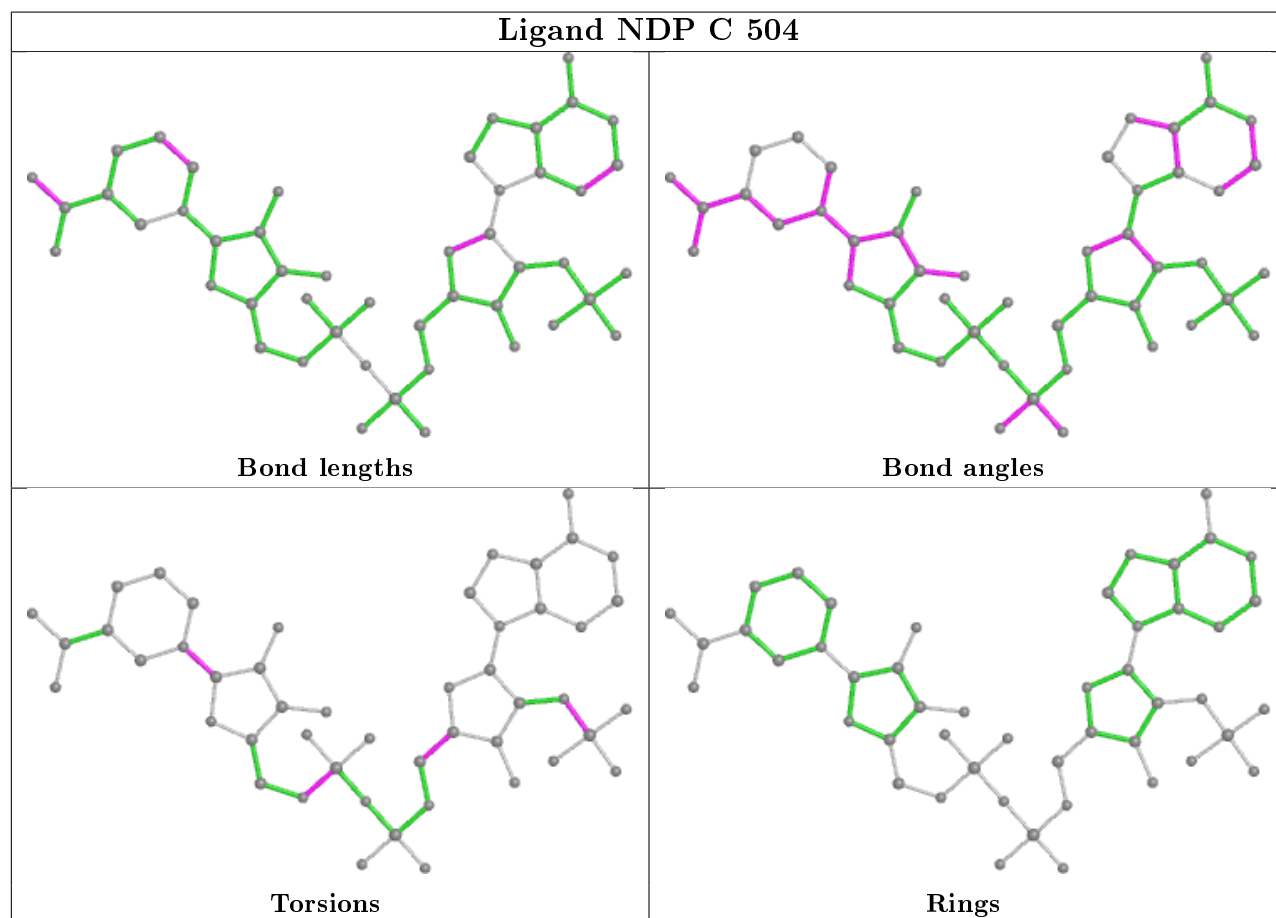
Mol	Chain	Res	Type	Atoms
3	C	504	NDP	C2B-O2B-P2B-O3X
3	C	504	NDP	C5D-O5D-PN-O1N
3	B	503	NDP	C5D-O5D-PN-O1N
3	A	501	NDP	C5D-O5D-PN-O1N
3	D	502	NDP	C5D-O5D-PN-O1N
3	C	504	NDP	O4D-C1D-N1N-C6N
3	B	503	NDP	C2B-O2B-P2B-O3X
3	B	503	NDP	C5D-O5D-PN-O3
3	D	502	NDP	C2B-O2B-P2B-O3X
3	B	503	NDP	O4D-C1D-N1N-C6N
3	D	502	NDP	O4D-C1D-N1N-C6N
3	C	504	NDP	C5D-O5D-PN-O2N
3	B	503	NDP	C5D-O5D-PN-O2N
3	A	501	NDP	C5D-O5D-PN-O2N
3	D	502	NDP	C5D-O5D-PN-O2N
3	A	501	NDP	O4D-C1D-N1N-C6N
3	B	503	NDP	O4B-C4B-C5B-O5B
3	C	504	NDP	C5D-O5D-PN-O3
3	A	501	NDP	C5D-O5D-PN-O3
3	D	502	NDP	C5D-O5D-PN-O3
3	C	504	NDP	O4B-C4B-C5B-O5B
3	A	501	NDP	O4B-C4B-C5B-O5B
3	D	502	NDP	O4B-C4B-C5B-O5B

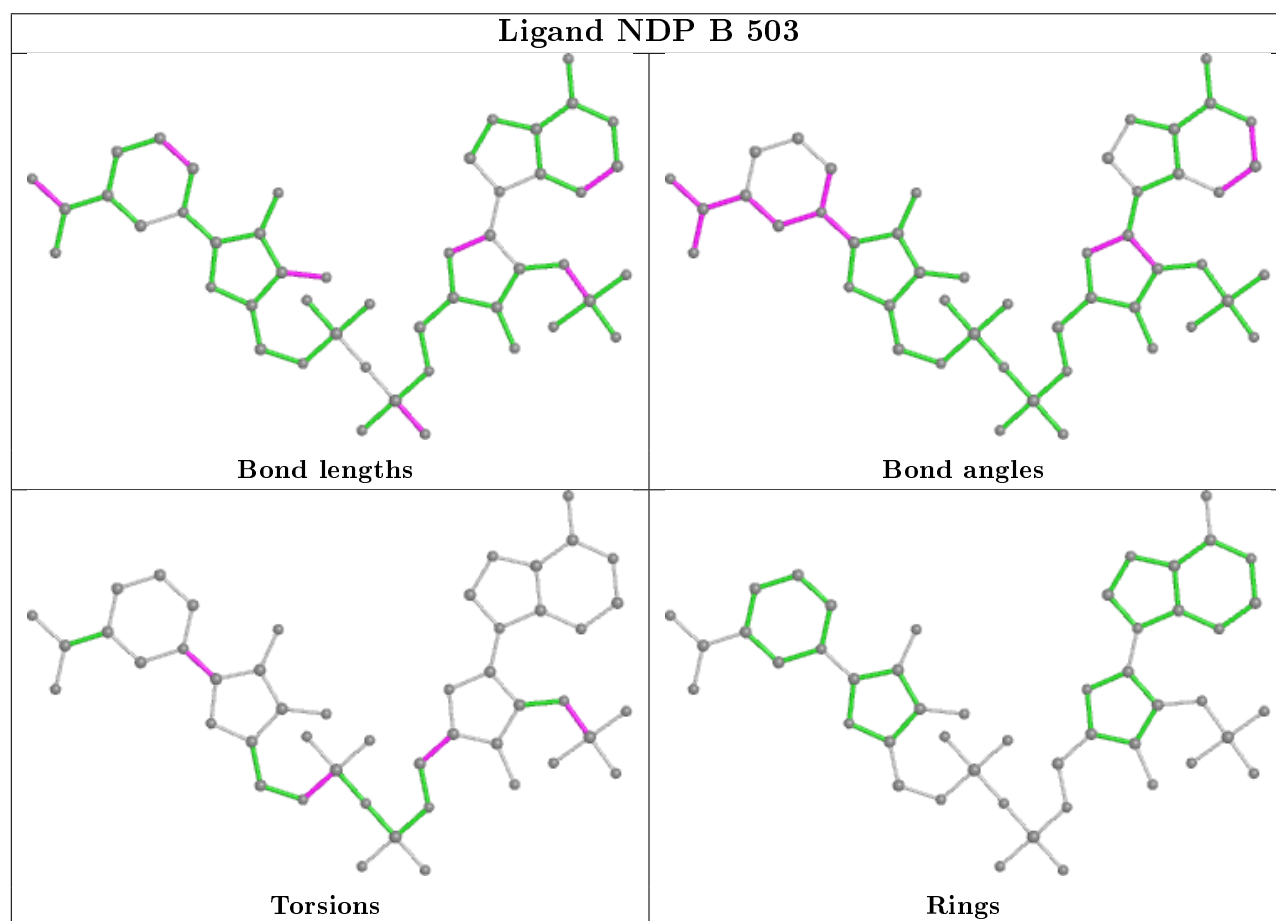
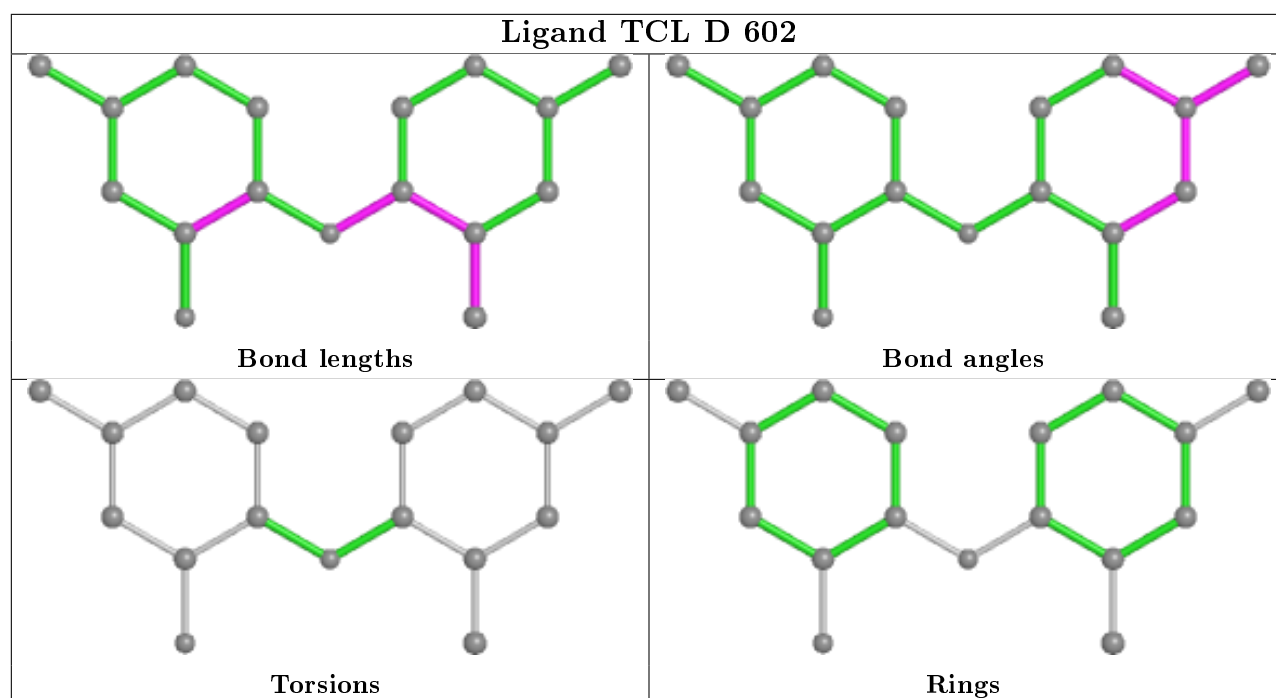
There are no ring outliers.

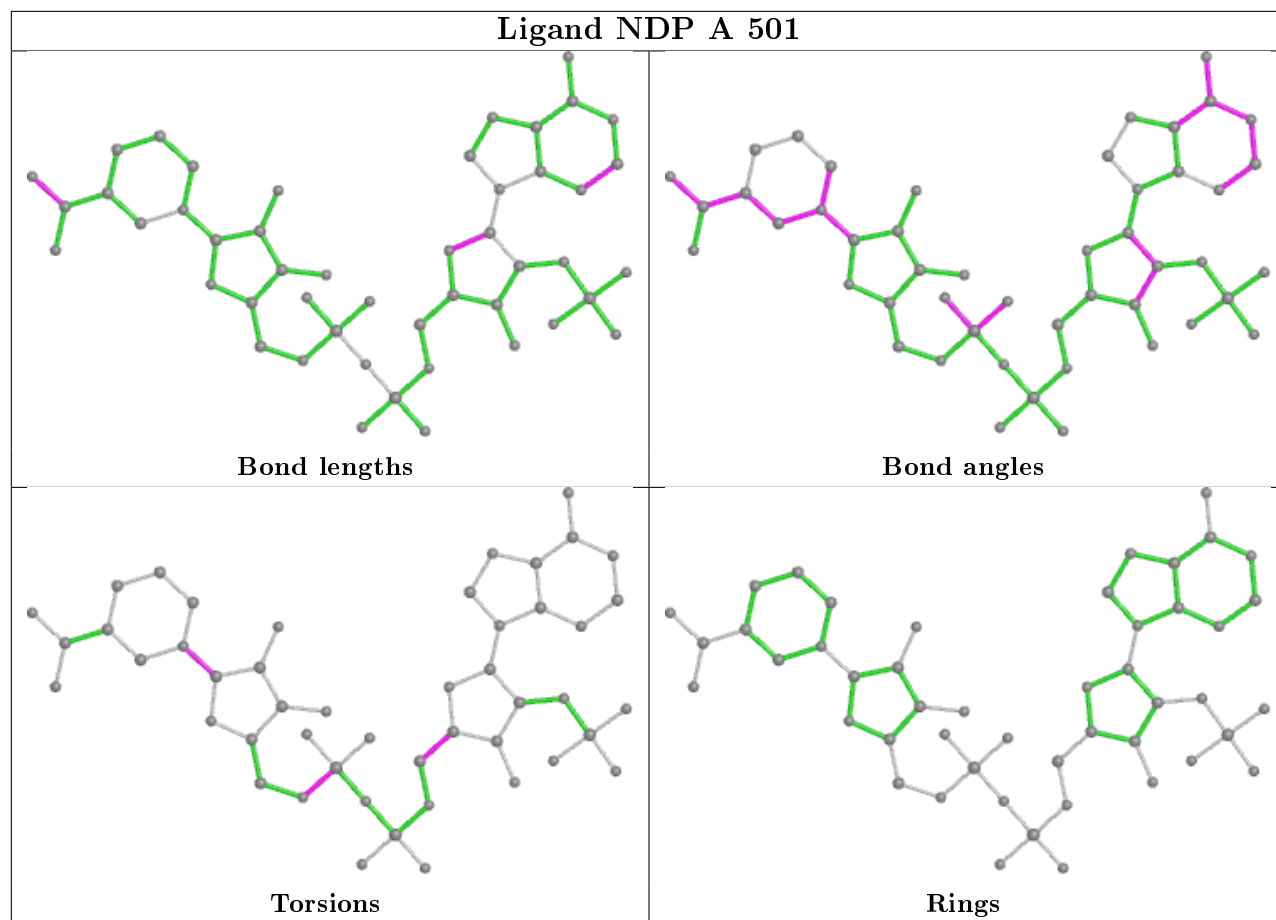
4 monomers are involved in 8 short contacts:

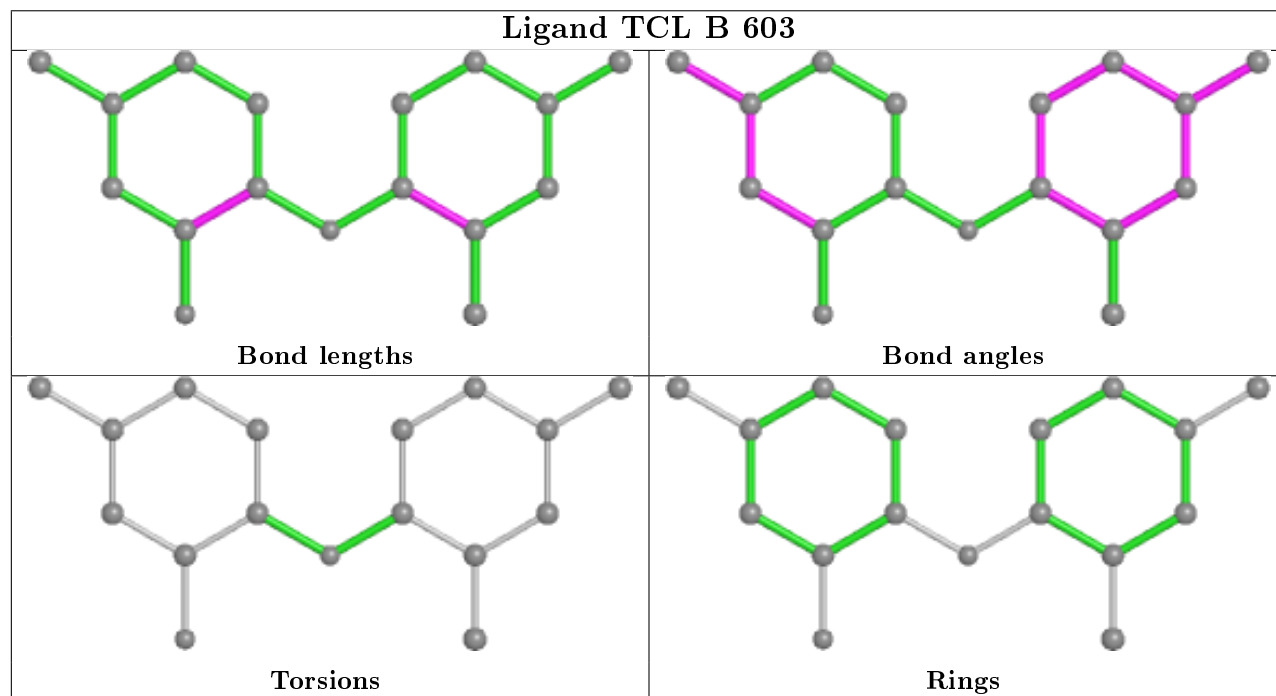
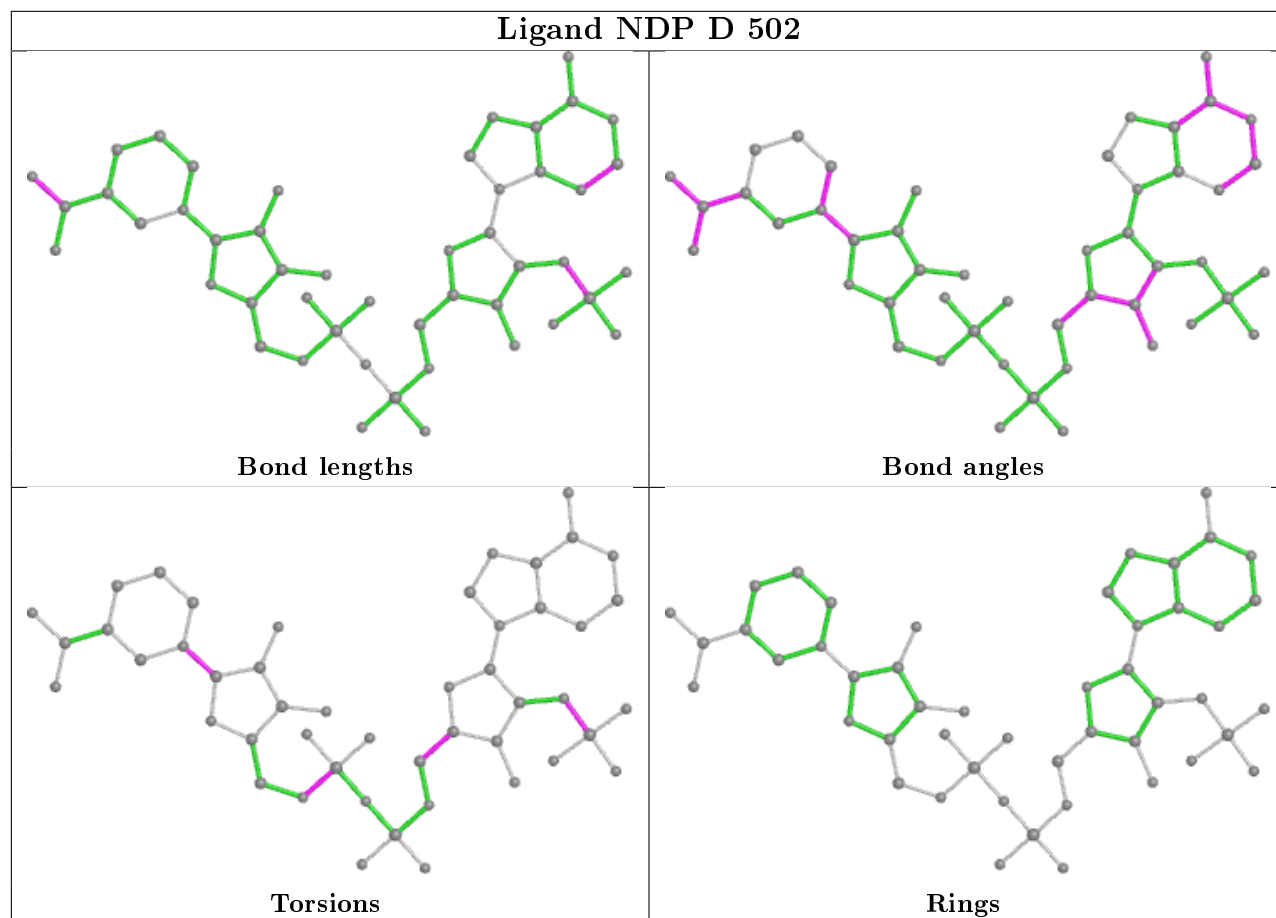
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	NDP	2	0
3	B	503	NDP	1	0
3	A	501	NDP	2	0
3	D	502	NDP	3	0

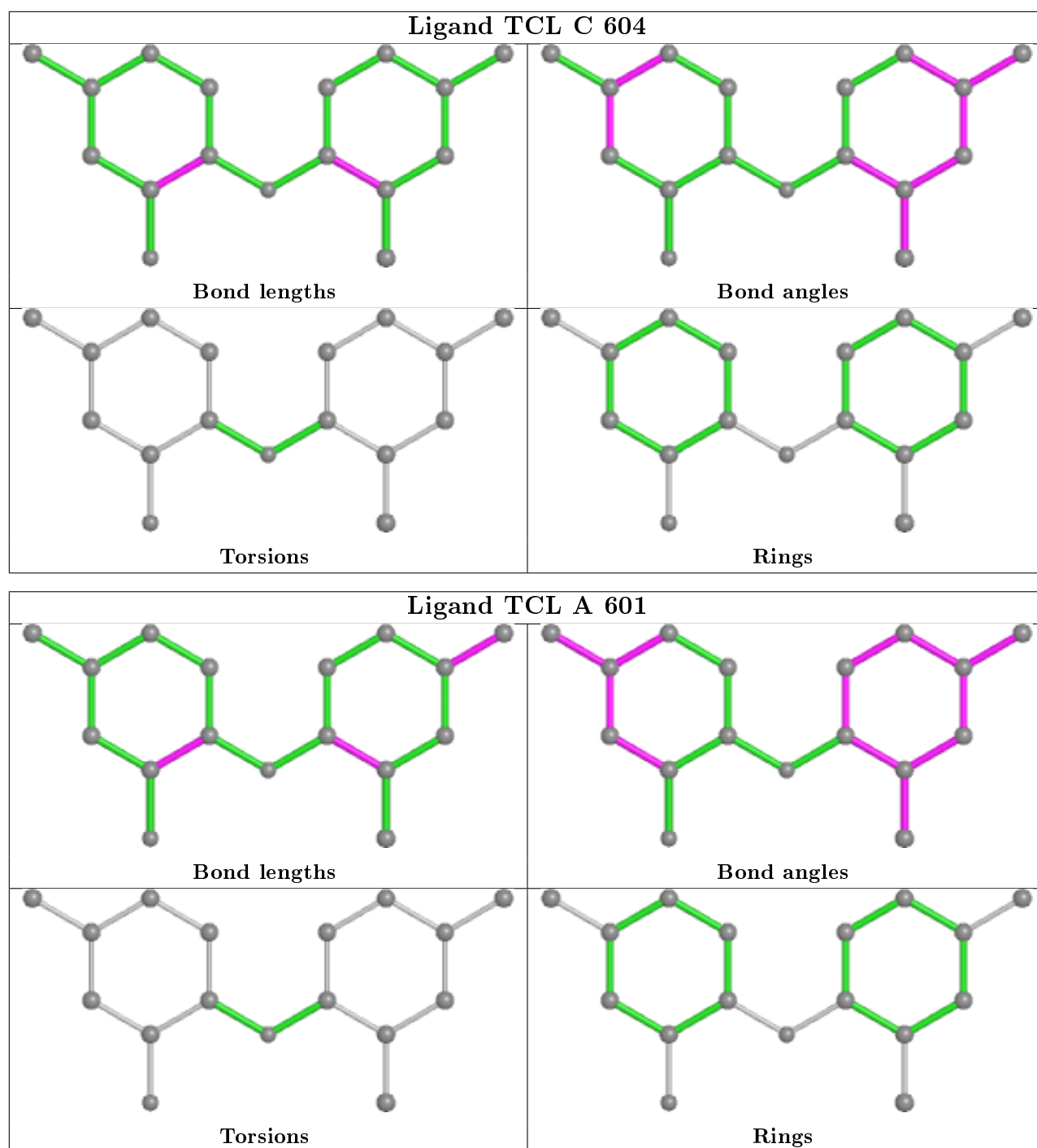
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	249/258 (96%)	-0.38	1 (0%) 92 90	7, 11, 26, 35	0
1	B	251/258 (97%)	-0.47	2 (0%) 86 84	6, 12, 25, 34	0
1	C	248/258 (96%)	-0.48	0 100 100	6, 13, 26, 35	0
1	D	248/258 (96%)	-0.40	0 100 100	7, 13, 28, 37	0
All	All	996/1032 (96%)	-0.43	3 (0%) 94 92	6, 12, 27, 37	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	LYS	2.6
1	A	203	GLU	2.6
1	B	47	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

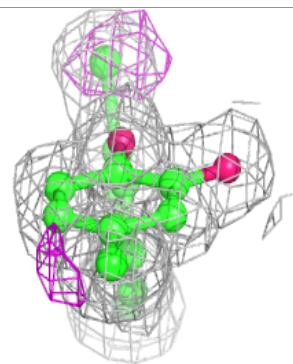
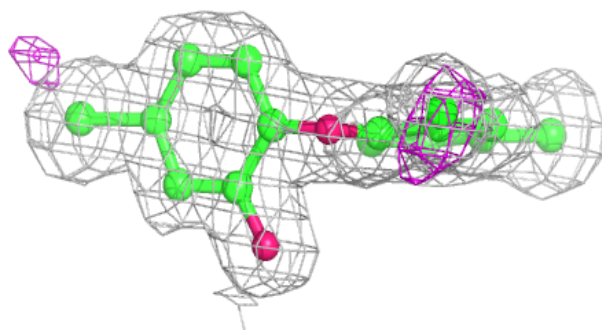
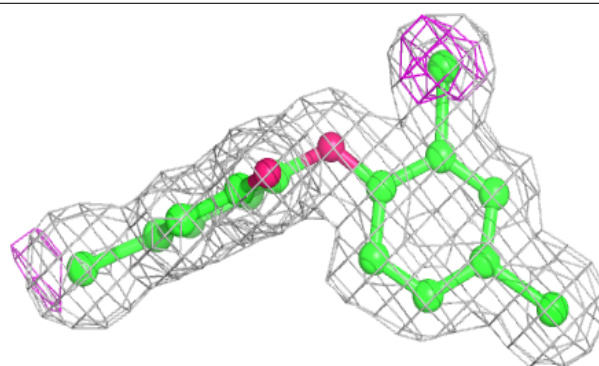
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TCL	B	603	17/17	0.97	0.07	10,12,22,23	0
2	TCL	C	604	17/17	0.97	0.07	10,14,23,24	0
3	NDP	B	503	48/48	0.98	0.06	6,10,14,17	0
3	NDP	C	504	48/48	0.98	0.06	7,11,14,17	0
2	TCL	D	602	17/17	0.98	0.07	9,13,23,23	0
2	TCL	A	601	17/17	0.98	0.07	10,13,21,23	0
3	NDP	D	502	48/48	0.99	0.06	8,11,13,15	0
3	NDP	A	501	48/48	0.99	0.06	6,9,13,13	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.

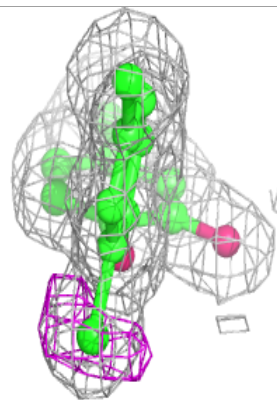
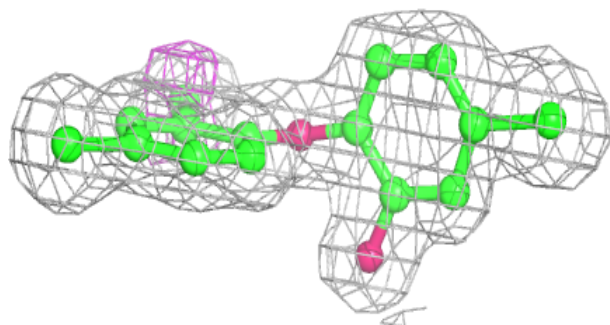
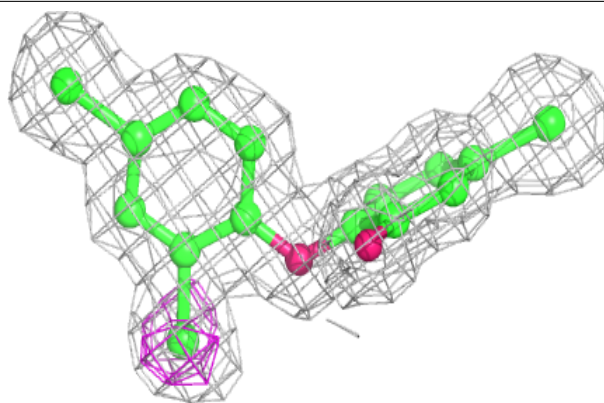
Electron density around TCL B 603:

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

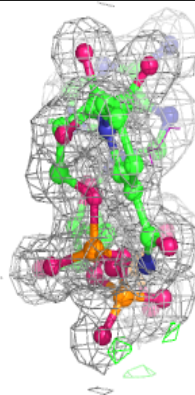
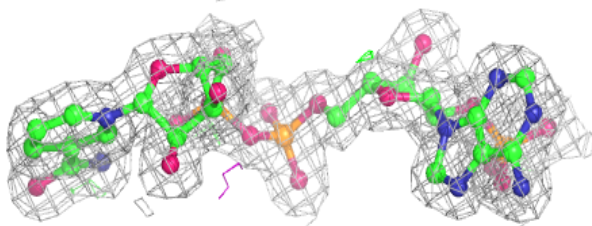
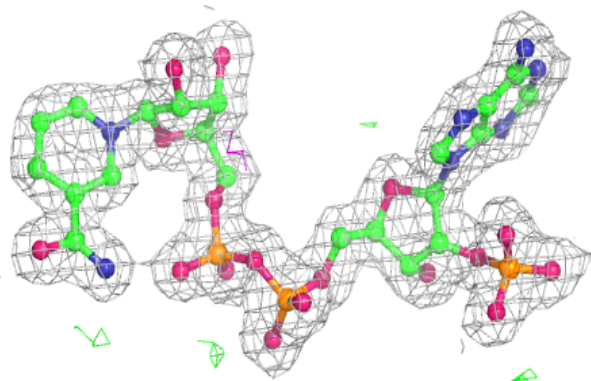


Electron density around TCL C 604:

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

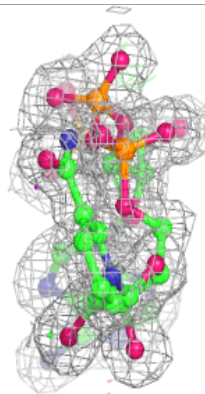
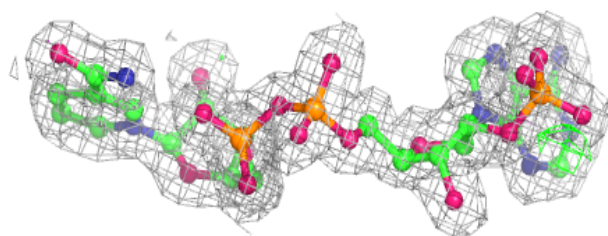
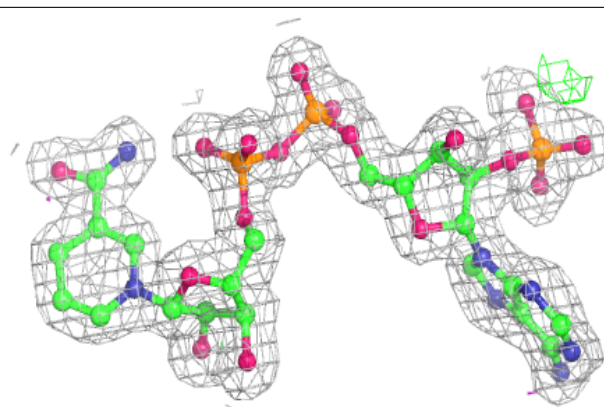
**Electron density around NDP B 503:**

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

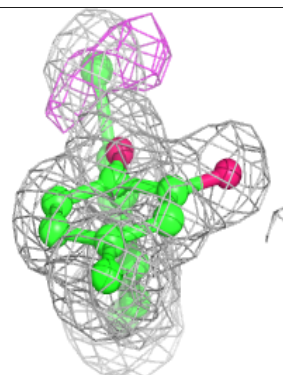
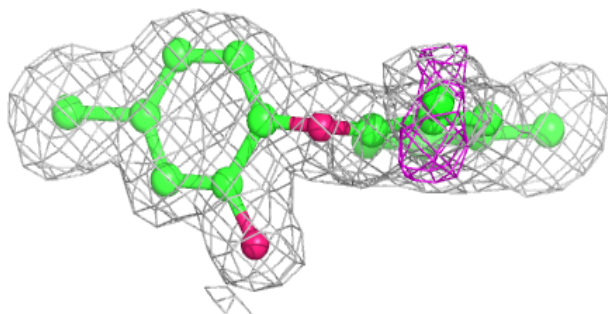
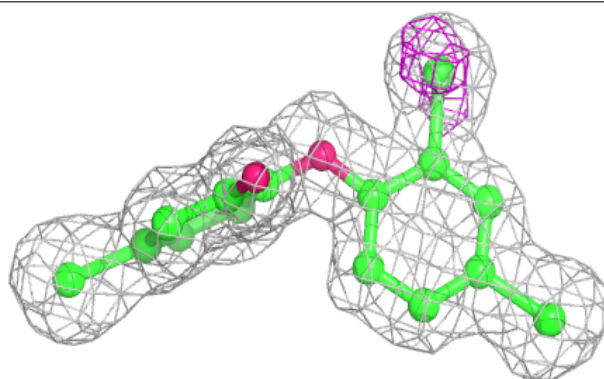


Electron density around NDP C 504:

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

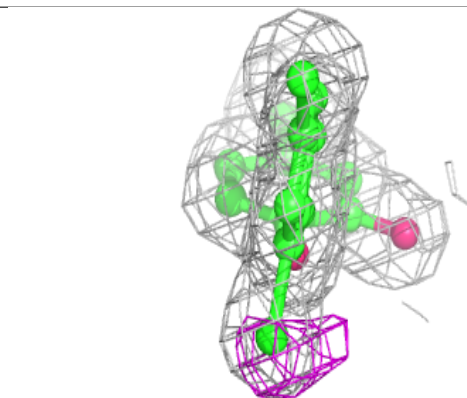
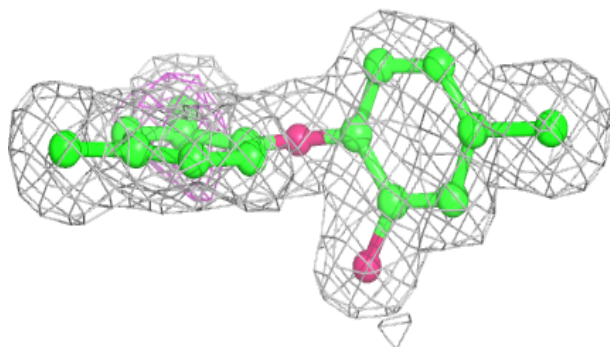
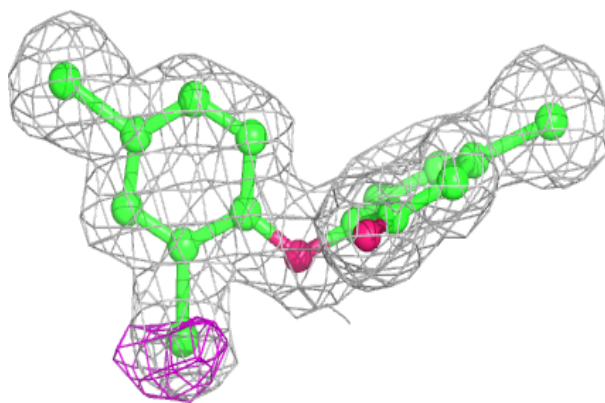
**Electron density around TCL D 602:**

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

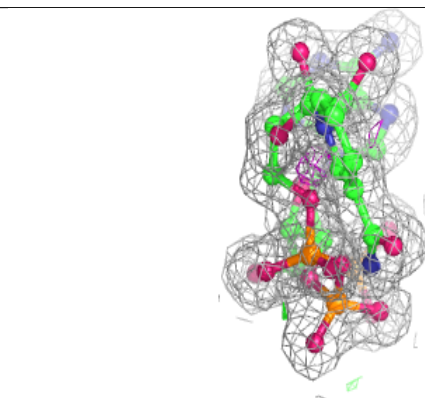
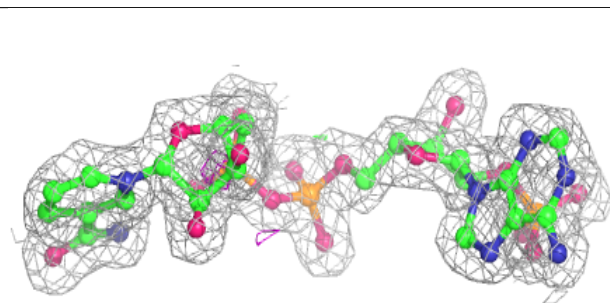
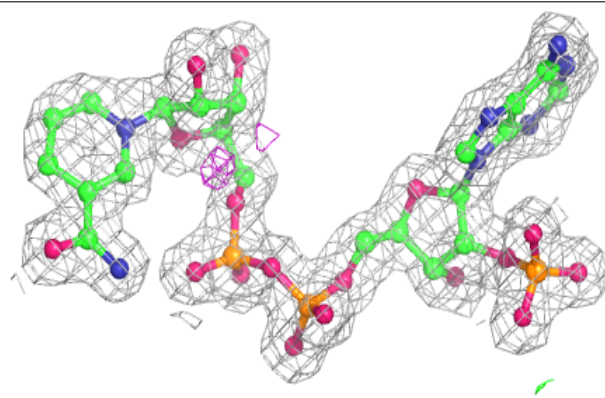


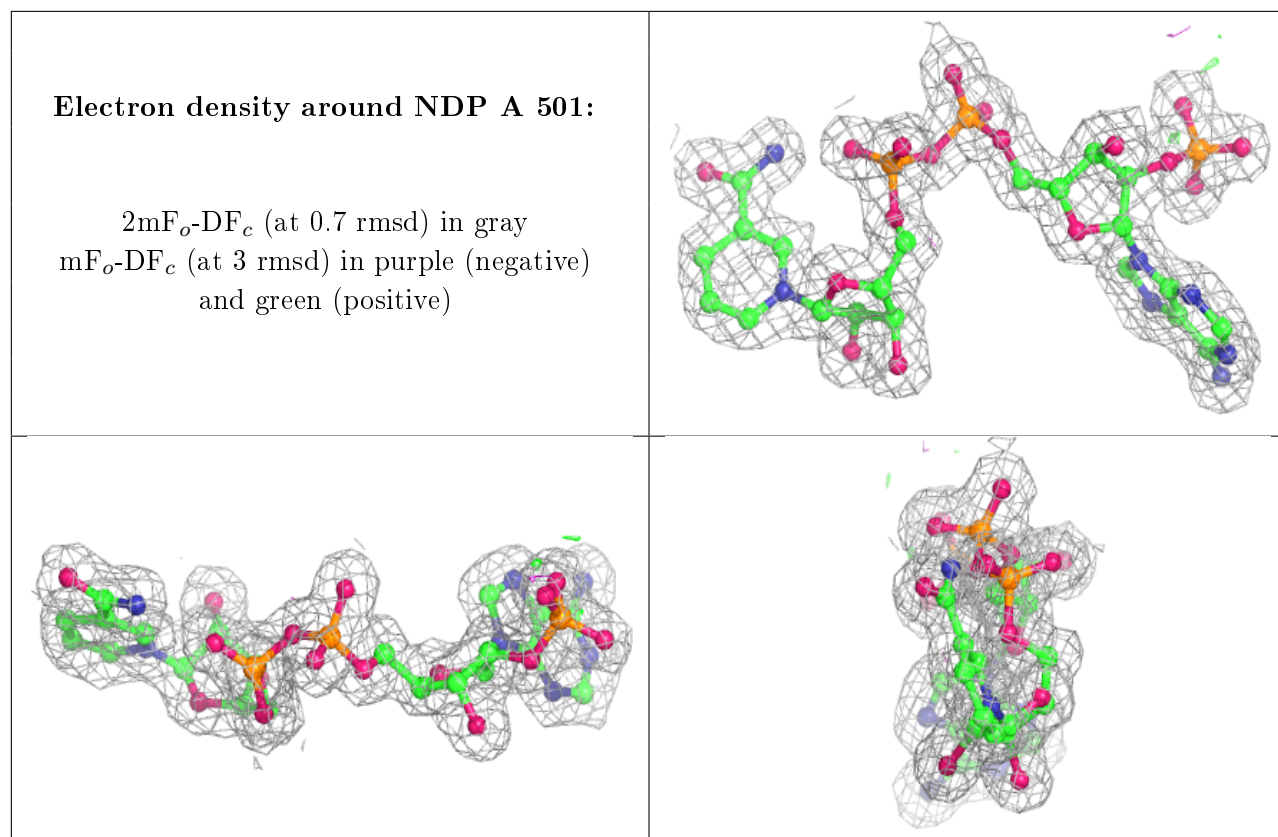
Electron density around TCL A 601:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.