



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 03:12 am BST

PDB ID : 4HX5
Title : Crystal structure of 11 beta-HSD1 in complex with SAR184841
Authors : Loenze, P.; Schimanski-Breves, S.; Engel, C.K.
Deposited on : 2012-11-09
Resolution : 2.19 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

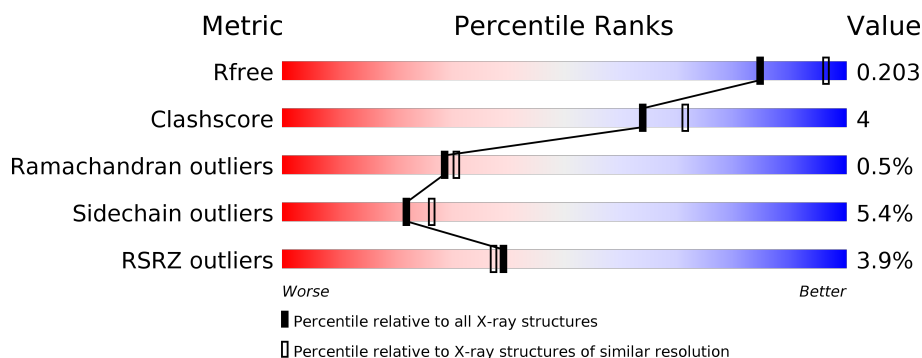
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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 ≥ 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	286	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	286	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>8%</div> </div> </div>
1	C	286	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>
1	D	286	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8877 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	1	0
			2008	1280	339	374	15			
1	B	264	Total	C	N	O	S	0	3	0
			2046	1303	349	379	15			
1	C	264	Total	C	N	O	S	0	1	0
			2036	1299	345	377	15			
1	D	260	Total	C	N	O	S	0	1	0
			2002	1276	342	369	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P28845
A	8	LYS	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	GLN	-	EXPRESSION TAG	UNP P28845
A	11	HIS	-	EXPRESSION TAG	UNP P28845
A	12	GLN	-	EXPRESSION TAG	UNP P28845
A	13	HIS	-	EXPRESSION TAG	UNP P28845
A	14	GLN	-	EXPRESSION TAG	UNP P28845
A	15	HIS	-	EXPRESSION TAG	UNP P28845
A	16	GLN	-	EXPRESSION TAG	UNP P28845
A	17	HIS	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	GLN	-	EXPRESSION TAG	UNP P28845
A	21	GLN	-	EXPRESSION TAG	UNP P28845
A	22	PRO	-	EXPRESSION TAG	UNP P28845
A	23	LEU	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED MUTATION	UNP P28845
B	7	MET	-	EXPRESSION TAG	UNP P28845
B	8	LYS	-	EXPRESSION TAG	UNP P28845
B	9	HIS	-	EXPRESSION TAG	UNP P28845

Continued on next page...

Continued from previous page...

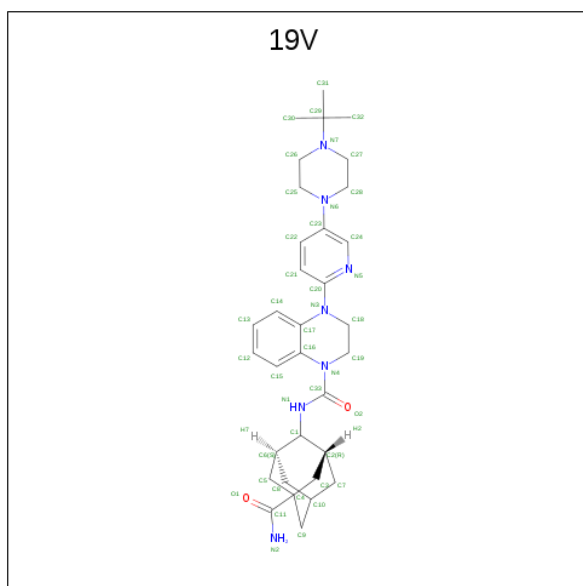
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
B	17	HIS	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	GLN	-	EXPRESSION TAG	UNP P28845
B	21	GLN	-	EXPRESSION TAG	UNP P28845
B	22	PRO	-	EXPRESSION TAG	UNP P28845
B	23	LEU	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED MUTATION	UNP P28845
C	7	MET	-	EXPRESSION TAG	UNP P28845
C	8	LYS	-	EXPRESSION TAG	UNP P28845
C	9	HIS	-	EXPRESSION TAG	UNP P28845
C	10	GLN	-	EXPRESSION TAG	UNP P28845
C	11	HIS	-	EXPRESSION TAG	UNP P28845
C	12	GLN	-	EXPRESSION TAG	UNP P28845
C	13	HIS	-	EXPRESSION TAG	UNP P28845
C	14	GLN	-	EXPRESSION TAG	UNP P28845
C	15	HIS	-	EXPRESSION TAG	UNP P28845
C	16	GLN	-	EXPRESSION TAG	UNP P28845
C	17	HIS	-	EXPRESSION TAG	UNP P28845
C	18	GLN	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	GLN	-	EXPRESSION TAG	UNP P28845
C	21	GLN	-	EXPRESSION TAG	UNP P28845
C	22	PRO	-	EXPRESSION TAG	UNP P28845
C	23	LEU	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED MUTATION	UNP P28845
D	7	MET	-	EXPRESSION TAG	UNP P28845
D	8	LYS	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	GLN	-	EXPRESSION TAG	UNP P28845
D	11	HIS	-	EXPRESSION TAG	UNP P28845
D	12	GLN	-	EXPRESSION TAG	UNP P28845
D	13	HIS	-	EXPRESSION TAG	UNP P28845
D	14	GLN	-	EXPRESSION TAG	UNP P28845
D	15	HIS	-	EXPRESSION TAG	UNP P28845

Continued on next page...

Continued from previous page...

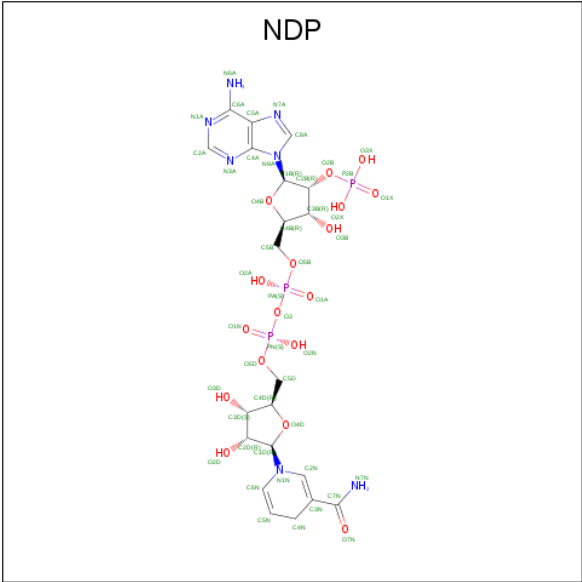
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED MUTATION	UNP P28845

- Molecule 2 is 4-[5-(4-tert-butylpiperazin-1-yl)pyridin-2-yl]-N-[(1R,2S,3S,5S,7s)-5-carbamoyl tricyclo[3.3.1.1 3,7]dec-2-yl]-3,4-dihydroquinoxaline-1(2H)-carboxamide (three-letter code: 19V) (formula: C₃₃H₄₅N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	33	7	2		
2	B	1	Total	C	N	O	0	0
			42	33	7	2		
2	C	1	Total	C	N	O	0	0
			42	33	7	2		
2	D	1	Total	C	N	O	0	0
			42	33	7	2		

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

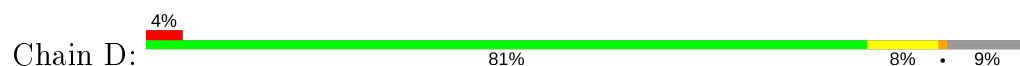
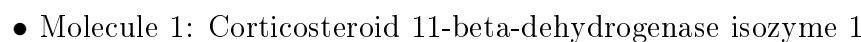
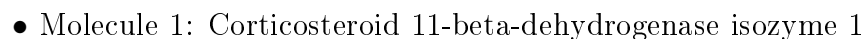
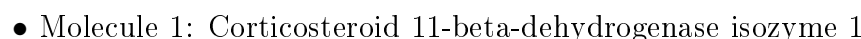


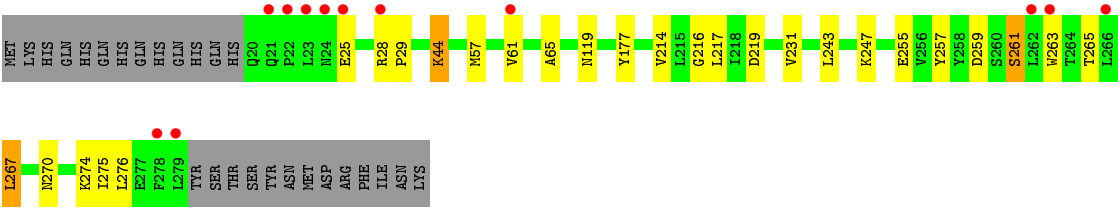
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total	O	0	0
			126	126		
4	B	103	Total	O	0	0
			103	103		
4	C	115	Total	O	0	0
			115	115		
4	D	81	Total	O	0	0
			81	81		

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.40Å 153.49Å 73.75Å 90.00° 92.89° 90.00°	Depositor
Resolution (Å)	73.66 – 2.19 56.33 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.66-2.19) 100.0 (56.33-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.18Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.163 , 0.199 0.166 , 0.203	Depositor DCC
R_{free} test set	3175 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8877	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 19V

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	0.48	0/2042	0.62	0/2757
1	B	0.48	0/2085	0.66	0/2816
1	C	0.48	0/2072	0.66	0/2799
1	D	0.46	0/2036	0.67	0/2749
All	All	0.47	0/8235	0.65	0/11121

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	2008	0	2050	16	0
1	B	2046	0	2088	32	0
1	C	2036	0	2078	12	0
1	D	2002	0	2051	16	0
2	A	42	0	45	2	0
2	B	42	0	45	11	0
2	C	42	0	45	3	0
2	D	42	0	45	6	0
3	A	48	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	0	0
3	C	48	0	26	0	0
3	D	48	0	26	2	0
4	A	126	0	0	2	0
4	B	103	0	0	2	0
4	C	115	0	0	1	0
4	D	81	0	0	0	0
All	All	8877	0	8551	72	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 4.

All (72) 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:262:LEU:N	1:B:263:TRP:HB2	1.78	0.98
1:B:177:TYR:HE2	2:B:301:19V:H16	1.37	0.88
1:B:261:SER:OG	1:B:263:TRP:HB3	1.76	0.85
1:B:177:TYR:CE2	2:B:301:19V:H16	2.12	0.85
1:B:262:LEU:H	1:B:263:TRP:HB2	1.39	0.83
1:D:177:TYR:HE2	2:D:301:19V:H16	1.45	0.81
1:B:266:LEU:HD11	1:D:275:ILE:HG13	1.61	0.80
1:B:261:SER:C	1:B:262:LEU:HG	2.03	0.79
1:C:231:VAL:HG21	2:C:301:19V:H40	1.65	0.77
1:D:177:TYR:CE2	2:D:301:19V:H16	2.19	0.77
1:B:261:SER:OG	1:B:263:TRP:CB	2.39	0.71
1:A:280:TYR:CD2	2:B:301:19V:H36	2.30	0.65
1:B:262:LEU:HB3	1:B:265:THR:OG1	1.99	0.63
1:B:261:SER:HB2	2:B:301:19V:H28	1.81	0.63
1:D:263:TRP:O	1:D:267:LEU:HB2	2.01	0.61
1:B:263:TRP:O	1:B:267:LEU:HB2	2.02	0.59
1:B:266:LEU:HD11	1:D:275:ILE:CG1	2.33	0.58
1:D:255:GLU:OE2	1:D:257:TYR:OH	2.14	0.58
1:B:140:MET:HB3	4:B:420:HOH:O	2.04	0.57
1:B:279:LEU:HD11	1:D:263:TRP:HE1	1.73	0.54
1:B:217:LEU:N	2:B:301:19V:N5	2.54	0.53
1:C:248:GLY:HA3	1:C:256:VAL:CG2	2.41	0.51
1:C:280:TYR:CD2	2:D:301:19V:H36	2.45	0.51
1:B:261:SER:C	1:B:262:LEU:CG	2.78	0.51
1:A:126:LEU:HD12	1:A:230:ILE:HG12	1.92	0.50
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:HE1	4:A:431:HOH:O	1.95	0.49
1:D:231:VAL:HG21	2:D:301:19V:H40	1.94	0.49
1:A:280:TYR:CD2	2:B:301:19V:H23	2.48	0.49
1:A:170:SER:OG	2:A:301:19V:H38	2.12	0.49
2:A:301:19V:C15	2:A:301:19V:H42	2.25	0.49
1:C:44:LYS:HB2	4:C:492:HOH:O	2.13	0.49
1:B:261:SER:HG	1:B:263:TRP:HB3	1.74	0.48
1:B:262:LEU:HB3	1:B:265:THR:CB	2.44	0.47
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.45	0.47
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.96	0.47
1:D:29:PRO:HB3	1:D:57:MET:HG2	1.97	0.47
1:B:261:SER:HB3	2:B:301:19V:H21	1.98	0.46
1:A:87:HIS:HD2	4:A:421:HOH:O	1.99	0.46
1:C:264:THR:O	1:C:268:ILE:HG13	2.16	0.46
1:D:119:ASN:ND2	3:D:302:NDP:H4D	2.31	0.45
1:B:170:SER:OG	2:B:301:19V:H38	2.16	0.45
1:A:280:TYR:CG	2:B:301:19V:H36	2.52	0.45
2:C:301:19V:H42	2:C:301:19V:C15	2.30	0.45
1:A:280:TYR:HD2	2:B:301:19V:H23	1.82	0.45
1:B:227:VAL:HB	1:B:231:VAL:HB	1.98	0.45
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.98	0.45
1:A:285:ASN:HD22	1:B:232:HIS:HE1	1.62	0.45
1:D:261:SER:HB3	2:D:301:19V:H21	1.99	0.44
1:B:141:GLU:HA	1:B:145:LEU:HB2	1.99	0.44
1:C:170:SER:OG	2:C:301:19V:H38	2.18	0.43
1:C:70:THR:O	1:C:74:VAL:HG23	2.18	0.43
1:C:216:GLY:HA3	1:C:259:ASP:OD2	2.18	0.43
1:B:216:GLY:HA3	1:B:259:ASP:OD2	2.18	0.43
1:B:262:LEU:N	1:B:263:TRP:CB	2.67	0.43
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.20	0.42
1:B:269:ARG:HG2	1:B:269:ARG:H	1.68	0.42
1:D:216:GLY:HA3	1:D:259:ASP:OD2	2.20	0.42
1:A:193:PHE:HB2	1:B:185:ALA:HB2	2.01	0.42
2:B:301:19V:C15	2:B:301:19V:H42	2.33	0.42
1:C:276:LEU:HD23	1:C:279:LEU:HD11	2.02	0.42
1:D:44:LYS:HG2	3:D:302:NDP:H3B	2.02	0.41
1:A:149:VAL:HG22	1:B:133:ILE:HD13	2.01	0.41
1:B:262:LEU:CA	1:B:263:TRP:HB2	2.46	0.41
1:D:217:LEU:N	2:D:301:19V:N5	2.61	0.41
1:D:214:VAL:HB	1:D:257:TYR:CD2	2.56	0.41
1:B:80:GLU:HG3	4:B:454:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ILE:HB	1:C:231:VAL:H	1.72	0.41
1:C:212:LEU:O	1:C:255:GLU:HA	2.21	0.40
1:D:243:LEU:HG	1:D:247:LYS:HE3	2.04	0.40
1:A:264:THR:O	1:A:268:ILE:HG13	2.22	0.40
1:B:279:LEU:HA	1:B:279:LEU:HD23	2.00	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	260/286 (91%)	250 (96%)	10 (4%)	0	100	100
1	B	265/286 (93%)	253 (96%)	11 (4%)	1 (0%)	34	37
1	C	263/286 (92%)	250 (95%)	11 (4%)	2 (1%)	19	19
1	D	259/286 (91%)	245 (95%)	12 (5%)	2 (1%)	19	19
All	All	1047/1144 (92%)	998 (95%)	44 (4%)	5 (0%)	29	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	TRP
1	C	230	ILE
1	D	219	ASP
1	C	219	ASP
1	D	65	ALA

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	219/243 (90%)	208 (95%)	11 (5%)	24	30
1	B	224/243 (92%)	213 (95%)	11 (5%)	25	31
1	C	222/243 (91%)	207 (93%)	15 (7%)	16	17
1	D	218/243 (90%)	208 (95%)	10 (5%)	27	34
All	All	883/972 (91%)	836 (95%)	47 (5%)	22	27

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LEU
1	A	160	GLN
1	A	202	SER
1	A	207	ASN
1	A	228	SER
1	A	230	ILE
1	A	231	VAL
1	A	234	GLN
1	A	262	LEU
1	A	270	ASN
1	A	274	LYS
1	B	28	ARG
1	B	68	LYS
1	B	225	LYS
1	B	234	GLN
1	B	261	SER
1	B	262	LEU
1	B	267	LEU
1	B	270	ASN
1	B	275	ILE
1	B	276	LEU
1	B	282	THR
1	C	24	ASN
1	C	26	GLU
1	C	61	VAL
1	C	69	GLU
1	C	70	THR
1	C	109	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	131	ASP
1	C	140	MET
1	C	145	LEU
1	C	230	ILE
1	C	234	GLN
1	C	239	GLU
1	C	266	LEU
1	C	270	ASN
1	C	279	LEU
1	D	25	GLU
1	D	28	ARG
1	D	44	LYS
1	D	61	VAL
1	D	261	SER
1	D	265	THR
1	D	267	LEU
1	D	270	ASN
1	D	274	LYS
1	D	276	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	105	GLN
1	A	119	ASN
1	A	270	ASN
1	B	119	ASN
1	B	127	ASN
1	B	232	HIS
1	B	270	ASN
1	C	87	HIS
1	C	119	ASN
1	C	270	ASN
1	D	77	HIS
1	D	87	HIS
1	D	119	ASN
1	D	127	ASN
1	D	270	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	$\# Z > 2$
2	19V	A	301	-	47,48,48	1.31	3 (6%)	66,74,74	1.62	10 (15%)
3	NDP	D	302	-	45,52,52	0.72	1 (2%)	53,80,80	0.96	3 (5%)
2	19V	C	301	-	47,48,48	1.34	5 (10%)	66,74,74	1.65	9 (13%)
3	NDP	C	302	-	45,52,52	0.69	1 (2%)	53,80,80	0.89	2 (3%)
3	NDP	A	302	-	45,52,52	0.62	0	53,80,80	0.87	4 (7%)
3	NDP	B	302	-	45,52,52	0.72	1 (2%)	53,80,80	0.91	3 (5%)
2	19V	B	301	-	47,48,48	1.47	6 (12%)	66,74,74	2.33	12 (18%)
2	19V	D	301	-	47,48,48	1.56	10 (21%)	66,74,74	1.80	12 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	19V	A	301	-	-	13/28/82/82	0/7/7/7
3	NDP	D	302	-	-	6/30/77/77	0/5/5/5
2	19V	C	301	-	-	4/28/82/82	0/7/7/7
3	NDP	C	302	-	-	2/30/77/77	0/5/5/5
3	NDP	A	302	-	-	4/30/77/77	0/5/5/5
3	NDP	B	302	-	-	4/30/77/77	0/5/5/5
2	19V	B	301	-	-	10/28/82/82	0/7/7/7
2	19V	D	301	-	-	6/28/82/82	0/7/7/7

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	19V	C17-N3	3.95	1.46	1.40
2	B	301	19V	C17-N3	3.70	1.46	1.40
2	B	301	19V	C28-N6	3.47	1.52	1.46
2	C	301	19V	C25-N6	3.17	1.51	1.46
2	D	301	19V	C26-N7	3.05	1.51	1.47
3	D	302	NDP	C6N-N1N	2.95	1.44	1.37
2	A	301	19V	C18-N3	2.80	1.51	1.46
2	D	301	19V	C20-N3	2.65	1.46	1.40
2	D	301	19V	C25-N6	2.56	1.50	1.46
2	A	301	19V	C25-N6	2.51	1.50	1.46
2	D	301	19V	C28-N6	2.50	1.50	1.46
2	A	301	19V	C17-N3	2.48	1.44	1.40
3	B	302	NDP	C6N-N1N	2.46	1.43	1.37
2	B	301	19V	C20-N3	2.44	1.45	1.40
2	B	301	19V	C5-C4	2.41	1.58	1.54
2	C	301	19V	C9-C4	2.34	1.58	1.54
2	C	301	19V	C18-N3	2.33	1.50	1.46
2	C	301	19V	C17-N3	2.32	1.44	1.40
2	D	301	19V	C23-N6	2.28	1.45	1.38
2	B	301	19V	C33-N4	-2.28	1.34	1.39
2	D	301	19V	C7-C2	2.20	1.58	1.53
3	C	302	NDP	P2B-O1X	-2.19	1.43	1.50
2	D	301	19V	C3-C4	2.17	1.58	1.54
2	D	301	19V	C8-C10	2.09	1.58	1.52
2	B	301	19V	C26-N7	2.05	1.50	1.47
2	D	301	19V	C18-N3	2.04	1.49	1.46
2	C	301	19V	C8-C10	2.03	1.58	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	19V	C26-N7-C29	11.60	121.62	113.74
2	B	301	19V	C27-N7-C29	8.30	119.38	113.74
2	D	301	19V	C26-N7-C29	7.59	118.90	113.74
2	C	301	19V	C26-N7-C29	7.13	118.58	113.74
2	A	301	19V	C26-N7-C29	6.75	118.33	113.74
2	C	301	19V	C27-N7-C29	5.15	117.24	113.74
2	A	301	19V	C28-N6-C25	4.77	122.05	111.52
2	A	301	19V	C18-C19-N4	-4.50	103.35	110.88
2	B	301	19V	C18-C19-N4	-4.47	103.39	110.88
2	D	301	19V	N1-C33-N4	4.46	120.53	114.04
2	C	301	19V	C28-N6-C25	4.45	121.35	111.52
2	D	301	19V	C18-C19-N4	-4.35	103.60	110.88
2	B	301	19V	C21-C20-N5	-4.04	116.00	123.41
2	A	301	19V	C27-N7-C29	4.04	116.49	113.74
2	C	301	19V	C18-C19-N4	-3.91	104.33	110.88
2	D	301	19V	C21-C20-N5	-3.89	116.28	123.41
2	B	301	19V	C24-N5-C20	3.79	124.22	117.30
2	B	301	19V	N5-C20-N3	3.77	124.35	116.15
2	D	301	19V	C24-N5-C20	3.63	123.92	117.30
2	B	301	19V	N1-C33-N4	3.61	119.29	114.04
2	D	301	19V	N5-C20-N3	3.54	123.85	116.15
2	C	301	19V	N1-C33-N4	3.18	118.66	114.04
2	D	301	19V	C22-C21-C20	3.05	121.73	117.53
2	A	301	19V	N1-C33-N4	2.92	118.28	114.04
3	D	302	NDP	O4D-C1D-N1N	2.89	113.70	108.06
2	C	301	19V	N5-C20-N3	2.88	122.42	116.15
2	C	301	19V	C24-N5-C20	2.87	122.53	117.30
2	D	301	19V	O2-C33-N4	-2.83	116.99	120.66
2	B	301	19V	C28-N6-C25	2.82	117.73	111.52
2	A	301	19V	C24-N5-C20	2.81	122.43	117.30
3	B	302	NDP	O2N-PN-O1N	2.78	125.97	112.24
2	B	301	19V	C22-C21-C20	2.71	121.26	117.53
2	B	301	19V	C17-N3-C20	2.68	124.98	120.38
2	C	301	19V	C21-C20-N5	-2.63	118.58	123.41
3	C	302	NDP	O2A-PA-O1A	2.63	125.24	112.24
2	A	301	19V	C21-C20-N5	-2.56	118.71	123.41
2	A	301	19V	N5-C20-N3	2.54	121.69	116.15
2	A	301	19V	C2-C1-N1	-2.48	107.27	112.00
2	D	301	19V	C28-N6-C25	2.48	116.99	111.52
3	B	302	NDP	C5A-C6A-N6A	2.46	124.08	120.35
3	C	302	NDP	C5A-C6A-N6A	2.40	124.00	120.35
2	D	301	19V	C25-N6-C23	2.33	124.38	118.09
2	B	301	19V	C15-C16-C17	2.29	122.92	118.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	19V	C27-N7-C26	2.27	112.02	109.06
3	D	302	NDP	C5A-C6A-N6A	2.24	123.76	120.35
3	D	302	NDP	O2N-PN-O1N	2.23	123.28	112.24
3	A	302	NDP	O2A-PA-O1A	2.20	123.11	112.24
3	A	302	NDP	C5A-C6A-N6A	2.14	123.61	120.35
2	A	301	19V	C22-C21-C20	2.10	120.43	117.53
2	C	301	19V	C22-C21-C20	2.09	120.41	117.53
2	D	301	19V	C27-N7-C26	2.07	111.76	109.06
3	B	302	NDP	O2A-PA-O1A	2.03	122.27	112.24
3	A	302	NDP	O2N-PN-O1N	2.02	122.24	112.24
3	A	302	NDP	O4D-C1D-N1N	2.02	112.00	108.06
2	D	301	19V	C17-N3-C20	2.01	123.83	120.38

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	19V	C21-C20-N3-C18
2	A	301	19V	N5-C20-N3-C18
2	A	301	19V	C31-C29-N7-C26
2	A	301	19V	C31-C29-N7-C27
2	A	301	19V	C32-C29-N7-C26
2	A	301	19V	C32-C29-N7-C27
2	A	301	19V	C30-C29-N7-C26
2	A	301	19V	C30-C29-N7-C27
3	D	302	NDP	C2B-O2B-P2B-O2X
2	C	301	19V	C21-C20-N3-C18
2	C	301	19V	N5-C20-N3-C18
2	B	301	19V	C21-C20-N3-C18
2	B	301	19V	N5-C20-N3-C18
2	B	301	19V	C31-C29-N7-C26
2	B	301	19V	C31-C29-N7-C27
2	B	301	19V	C32-C29-N7-C26
2	B	301	19V	C32-C29-N7-C27
2	B	301	19V	C30-C29-N7-C26
2	B	301	19V	C30-C29-N7-C27
2	D	301	19V	C21-C20-N3-C18
2	D	301	19V	N5-C20-N3-C18
2	A	301	19V	C22-C23-N6-C25
3	A	302	NDP	O4D-C1D-N1N-C6N
2	A	301	19V	C24-C23-N6-C25
2	D	301	19V	C31-C29-N7-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	301	19V	C21-C20-N3-C17
2	C	301	19V	C21-C20-N3-C17
2	B	301	19V	C21-C20-N3-C17
2	D	301	19V	C21-C20-N3-C17
3	C	302	NDP	O4D-C1D-N1N-C6N
3	B	302	NDP	O4D-C1D-N1N-C6N
2	A	301	19V	C22-C23-N6-C28
3	C	302	NDP	O4B-C4B-C5B-O5B
3	D	302	NDP	O4D-C1D-N1N-C6N
2	A	301	19V	C24-C23-N6-C28
2	D	301	19V	C32-C29-N7-C27
2	D	301	19V	C30-C29-N7-C27
3	A	302	NDP	C2B-O2B-P2B-O2X
3	B	302	NDP	PN-O3-PA-O1A
3	D	302	NDP	O4B-C4B-C5B-O5B
3	B	302	NDP	O4B-C4B-C5B-O5B
3	A	302	NDP	O4B-C4B-C5B-O5B
2	C	301	19V	N5-C20-N3-C17
2	B	301	19V	N5-C20-N3-C17
3	D	302	NDP	C2B-O2B-P2B-O1X
3	D	302	NDP	O4D-C4D-C5D-O5D
3	B	302	NDP	C2B-O2B-P2B-O2X
3	D	302	NDP	C2N-C3N-C7N-N7N
3	A	302	NDP	C2N-C3N-C7N-N7N

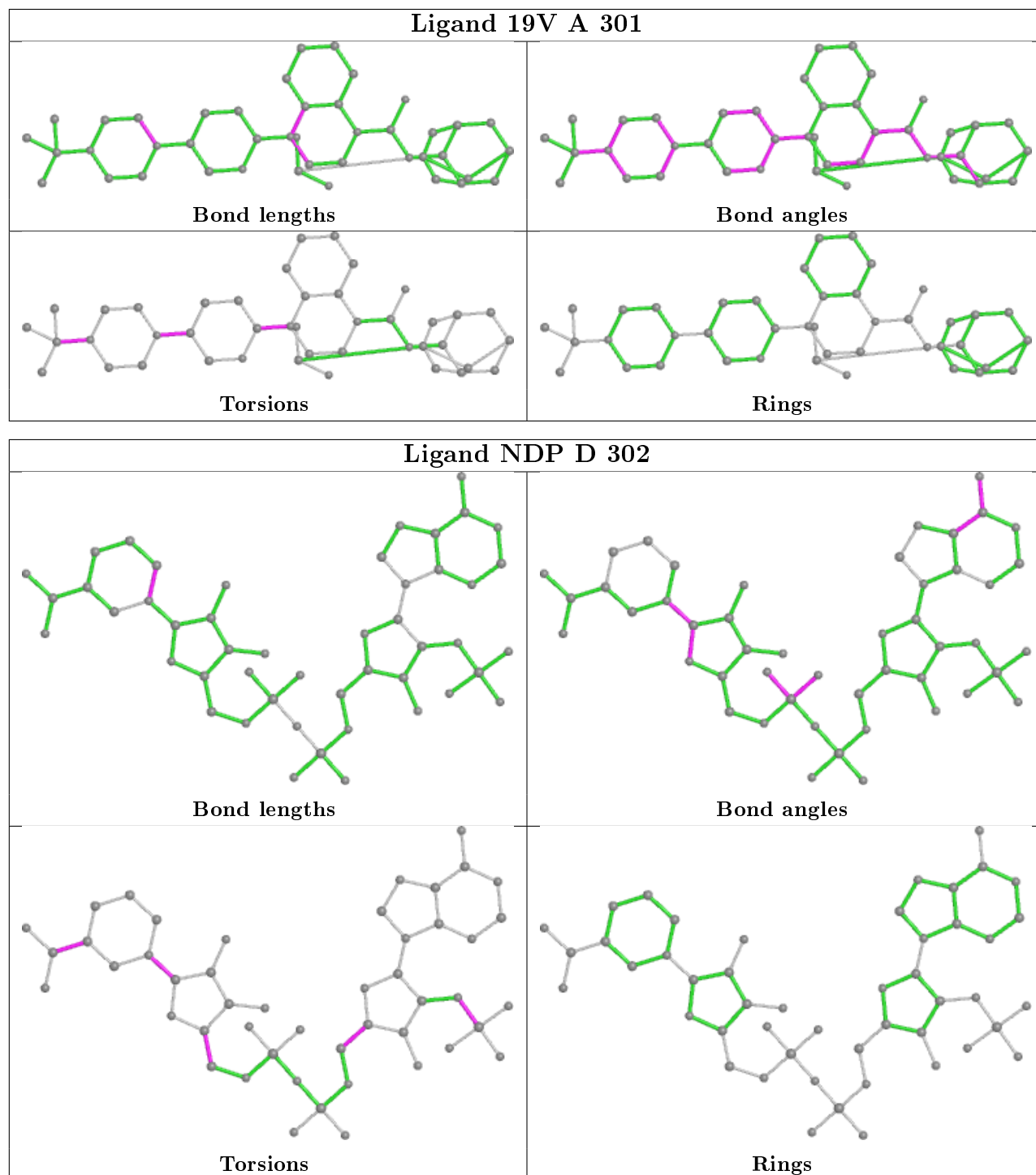
There are no ring outliers.

5 monomers are involved in 24 short contacts:

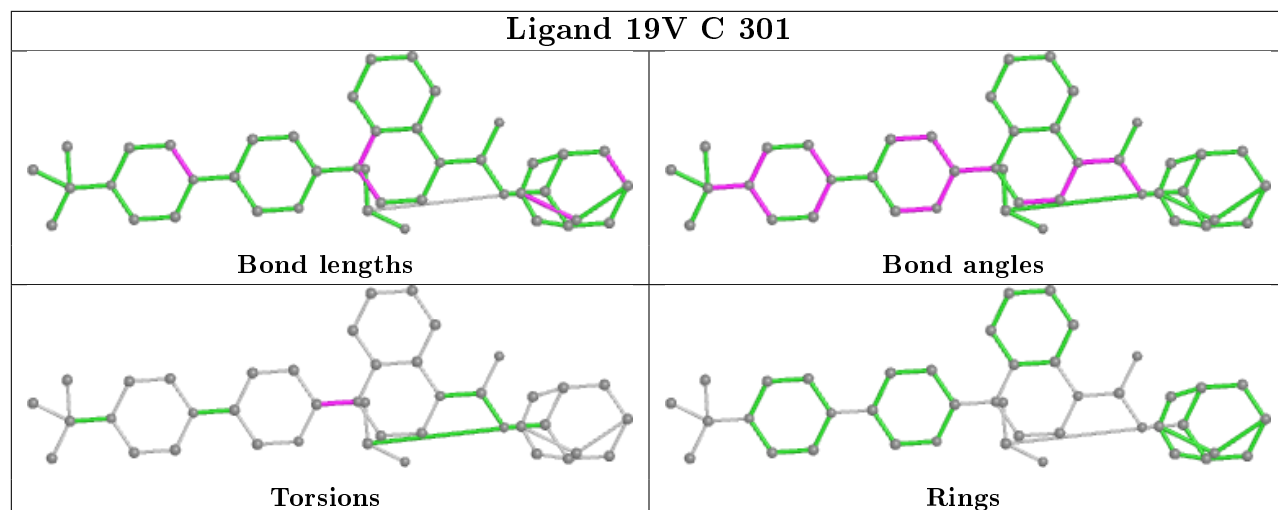
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	19V	2	0
3	D	302	NDP	2	0
2	C	301	19V	3	0
2	B	301	19V	11	0
2	D	301	19V	6	0

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

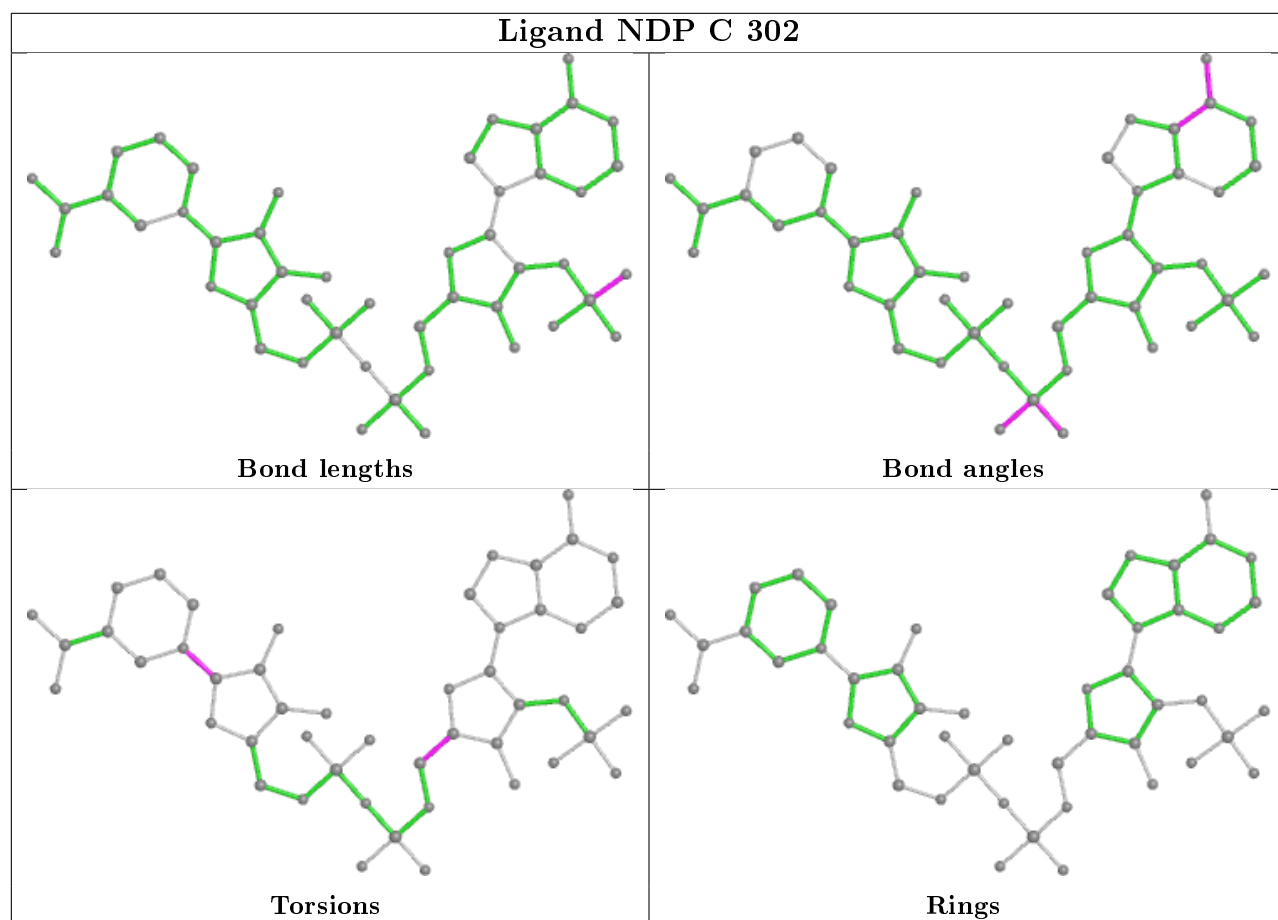
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

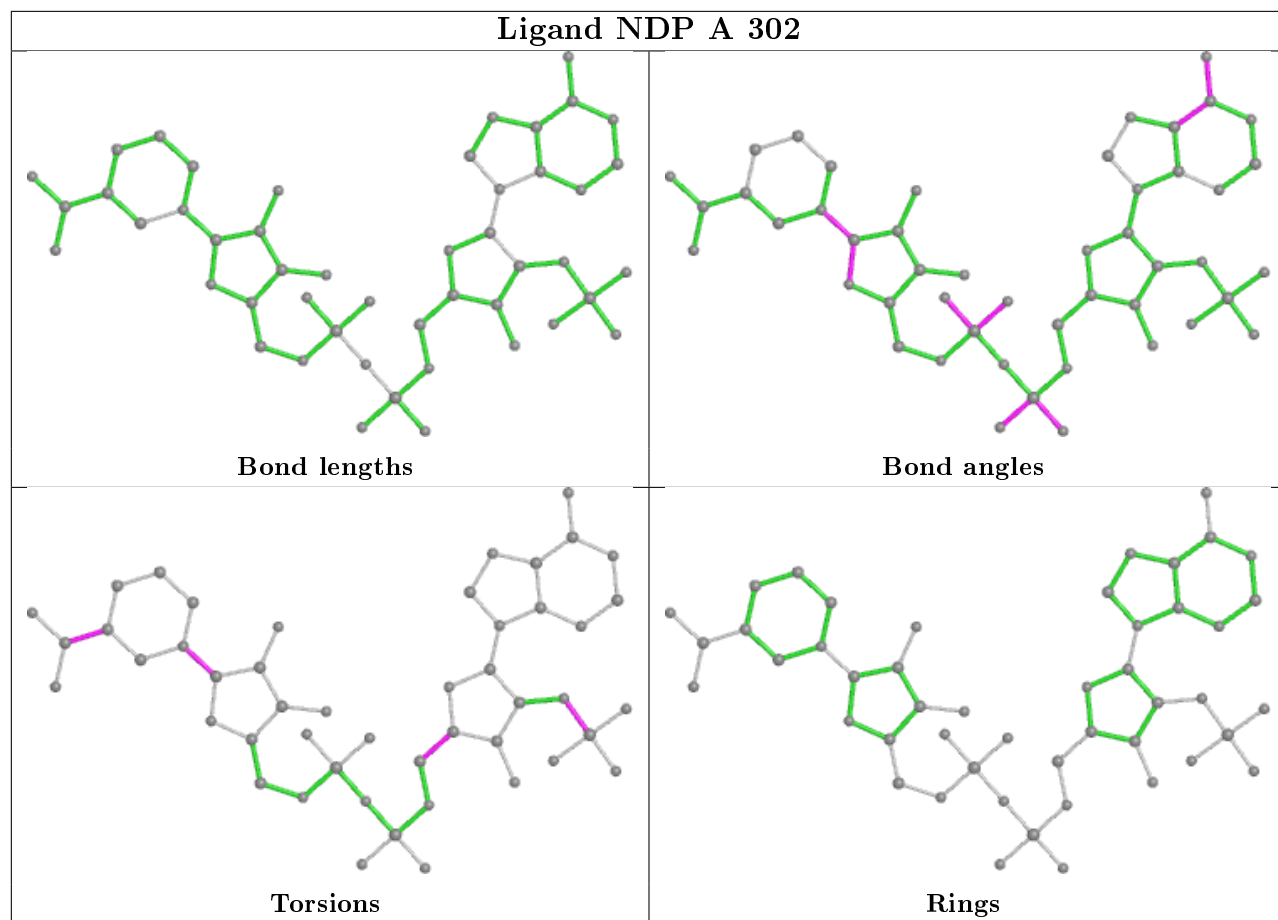


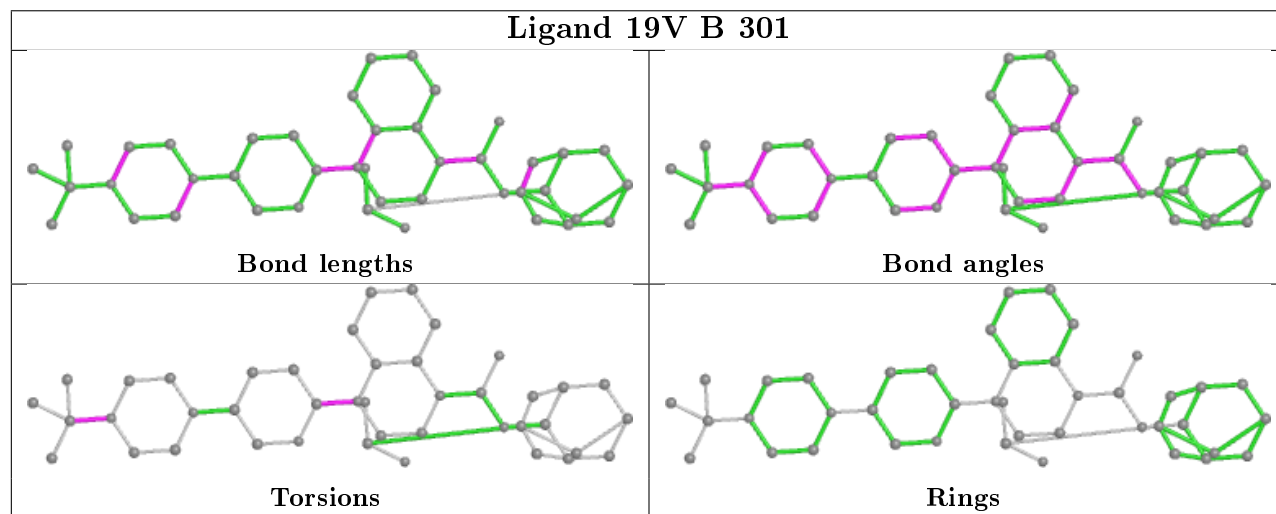
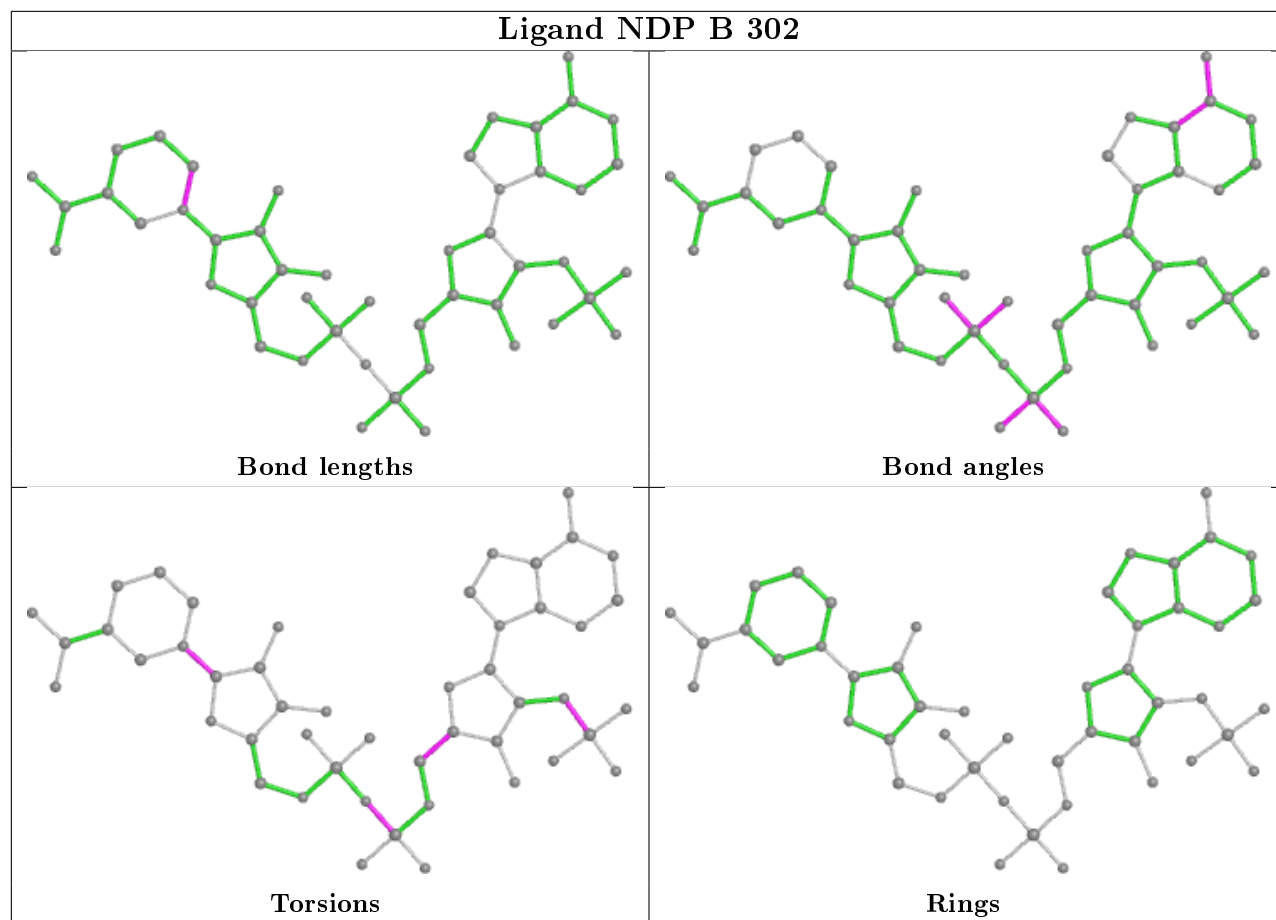
Ligand 19V C 301

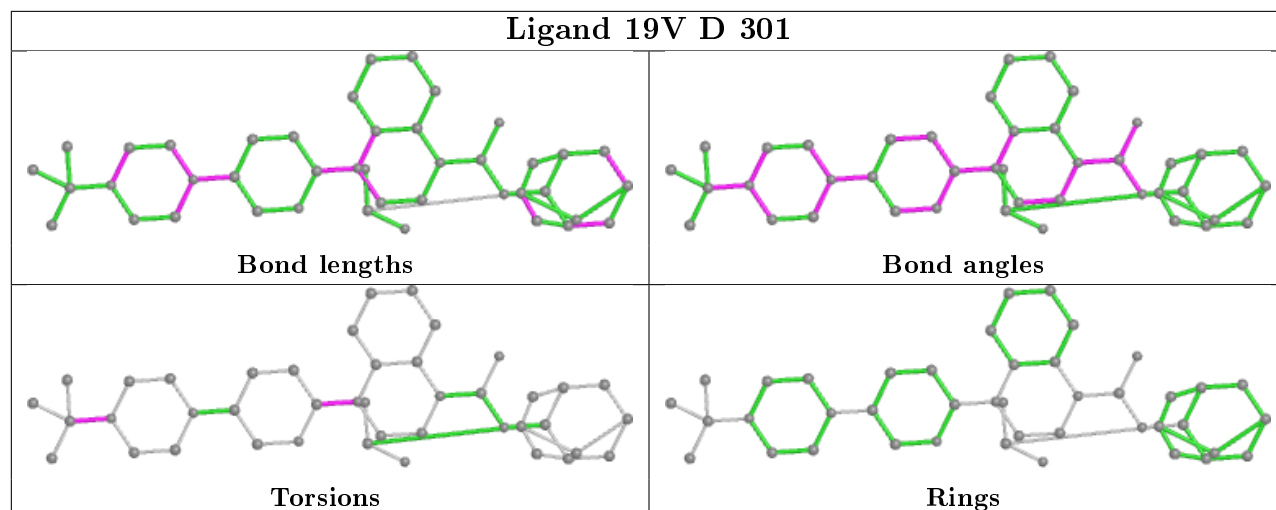


Ligand NDP C 302









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, 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	261/286 (91%)	-0.23	6 (2%) 60 58	12, 23, 48, 81	1 (0%)
1	B	264/286 (92%)	-0.10	12 (4%) 33 32	11, 24, 56, 87	0
1	C	264/286 (92%)	-0.26	11 (4%) 36 34	13, 21, 52, 74	1 (0%)
1	D	260/286 (90%)	0.08	12 (4%) 32 31	14, 30, 60, 85	0
All	All	1049/1144 (91%)	-0.12	41 (3%) 39 37	11, 25, 56, 87	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	LEU	7.0
1	B	24	ASN	6.4
1	C	24	ASN	5.7
1	D	24	ASN	5.5
1	B	280	TYR	5.4
1	B	262	LEU	5.4
1	D	262	LEU	4.4
1	B	23	LEU	4.2
1	A	25	GLU	3.8
1	A	263	TRP	3.7
1	A	229	GLY	3.6
1	C	21	GLN	3.5
1	D	22	PRO	3.2
1	C	279	LEU	3.2
1	D	266	LEU	3.1
1	D	263	TRP	3.0
1	C	231	VAL	3.0
1	D	278	PHE	3.0
1	A	232	HIS	3.0
1	D	25	GLU	3.0
1	B	263	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	21	GLN	2.9
1	B	20	GLN	2.9
1	C	280	TYR	2.8
1	C	263	TRP	2.7
1	B	21	GLN	2.7
1	C	22	PRO	2.7
1	B	232	HIS	2.6
1	B	278	PHE	2.6
1	C	230	ILE	2.4
1	C	23	LEU	2.4
1	C	232	HIS	2.3
1	B	279	LEU	2.3
1	D	28	ARG	2.2
1	B	282	THR	2.2
1	D	279	LEU	2.2
1	B	281	SER	2.1
1	C	130	HIS	2.1
1	A	262	LEU	2.1
1	D	61	VAL	2.1
1	A	230	ILE	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, 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	19V	B	301	42/42	0.88	0.20	16,23,71,73	0
2	19V	D	301	42/42	0.88	0.19	23,32,73,75	0
2	19V	A	301	42/42	0.91	0.17	18,30,56,57	0

Continued on next page...

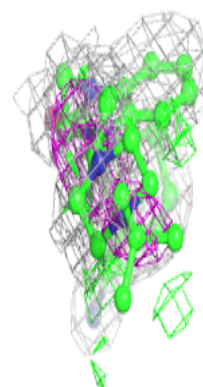
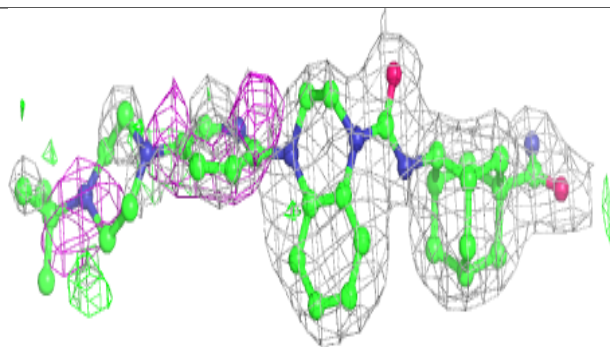
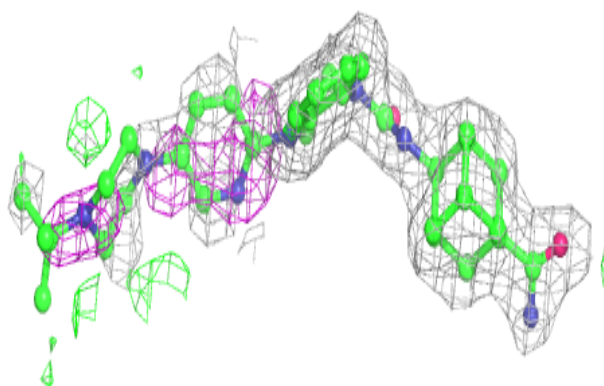
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	19V	C	301	42/42	0.95	0.13	19,29,44,46	0
3	NDP	D	302	48/48	0.98	0.08	17,22,28,33	0
3	NDP	B	302	48/48	0.99	0.11	13,18,22,24	0
3	NDP	C	302	48/48	0.99	0.09	13,16,20,22	0
3	NDP	A	302	48/48	0.99	0.09	13,16,20,23	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.

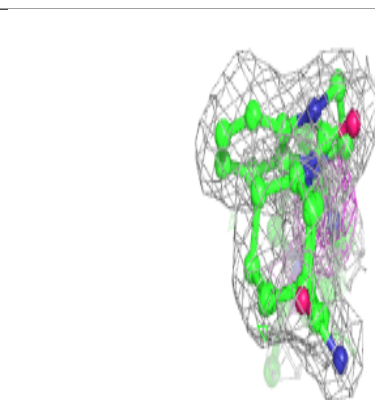
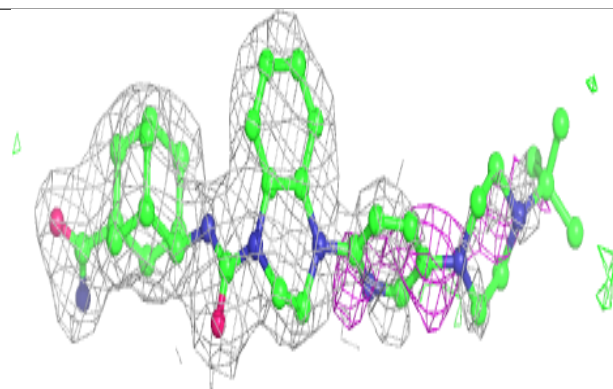
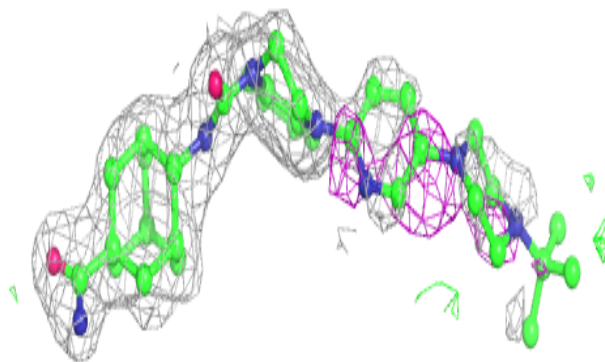
Electron density around 19V B 301:

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

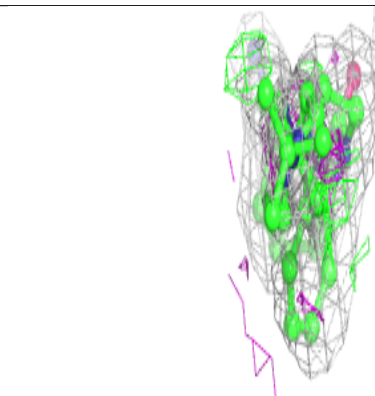
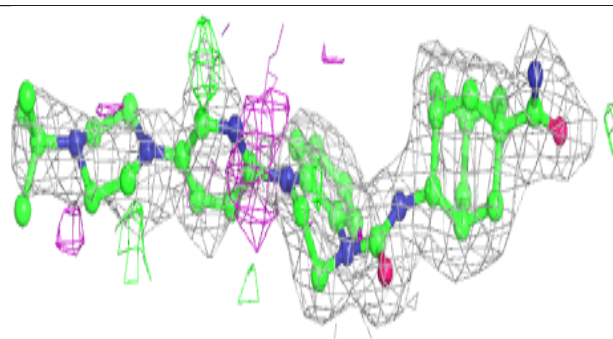
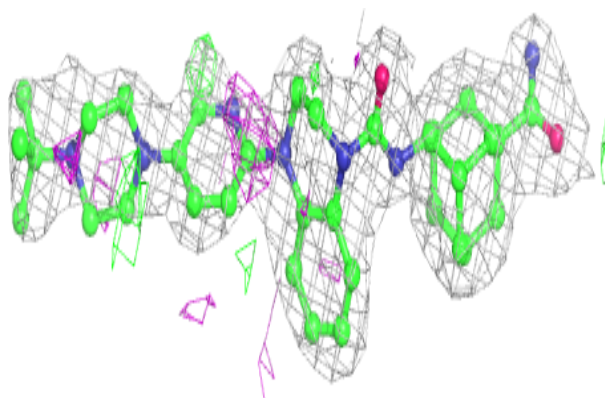


Electron density around 19V D 301:

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

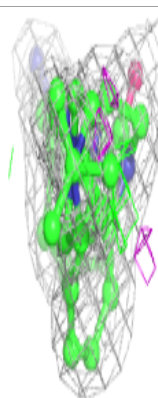
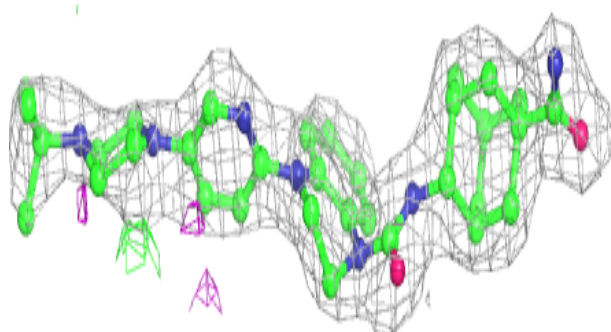
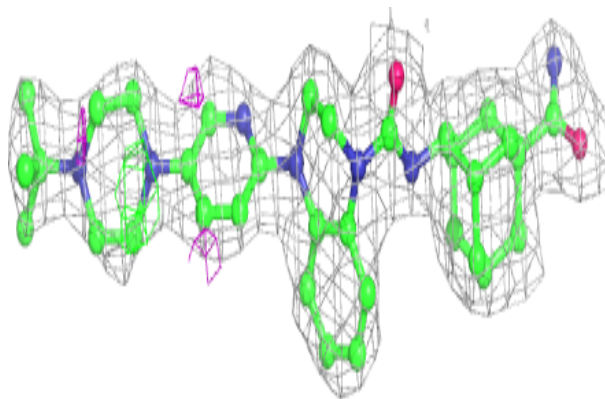
**Electron density around 19V A 301:**

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

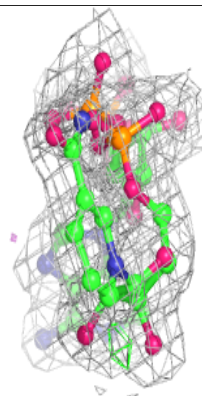
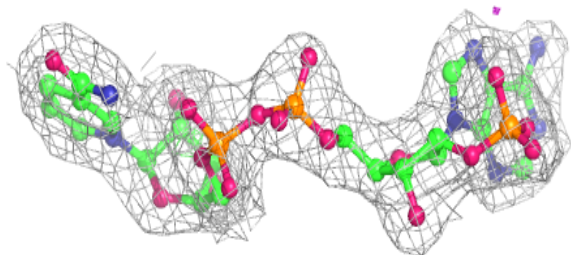
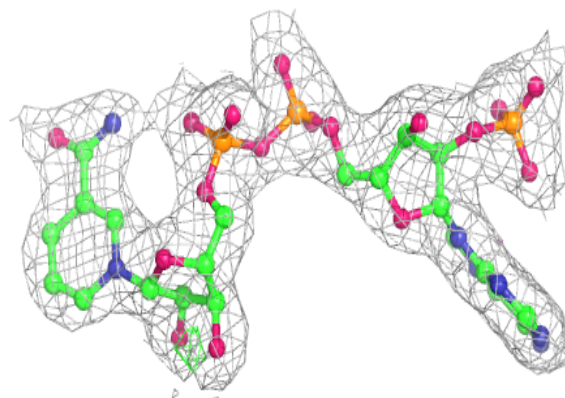


Electron density around 19V C 301:

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

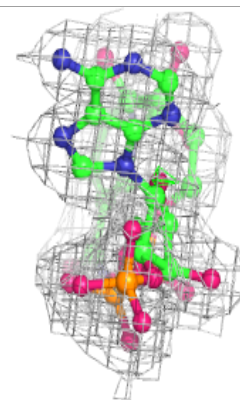
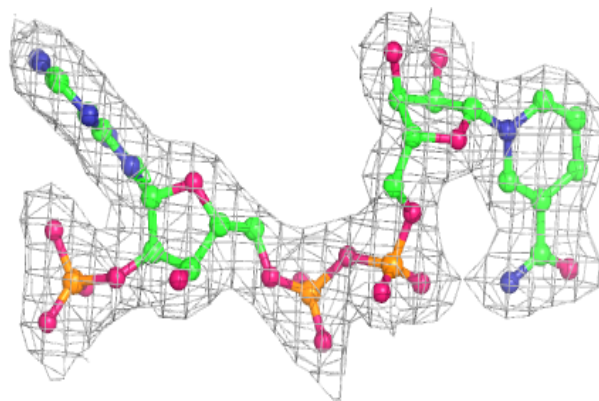
**Electron density around NDP D 302:**

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

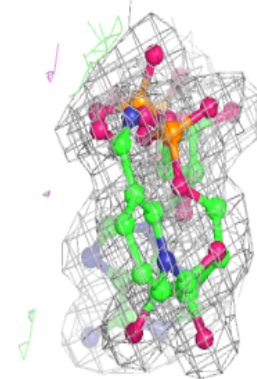
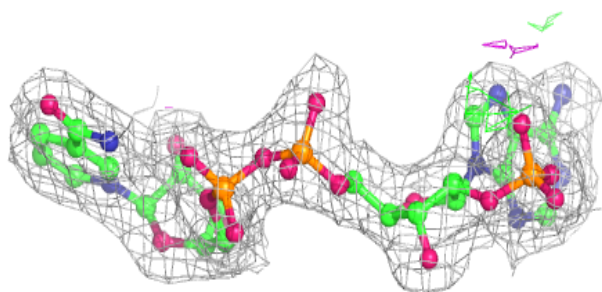
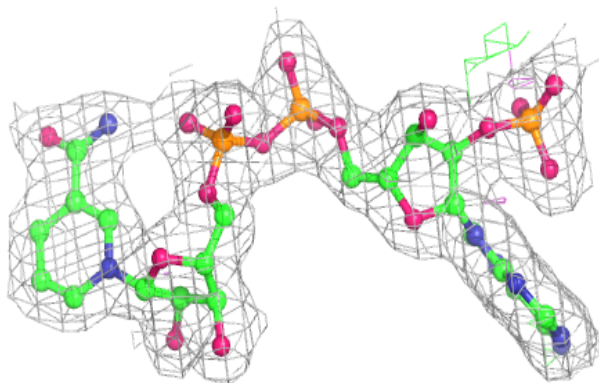


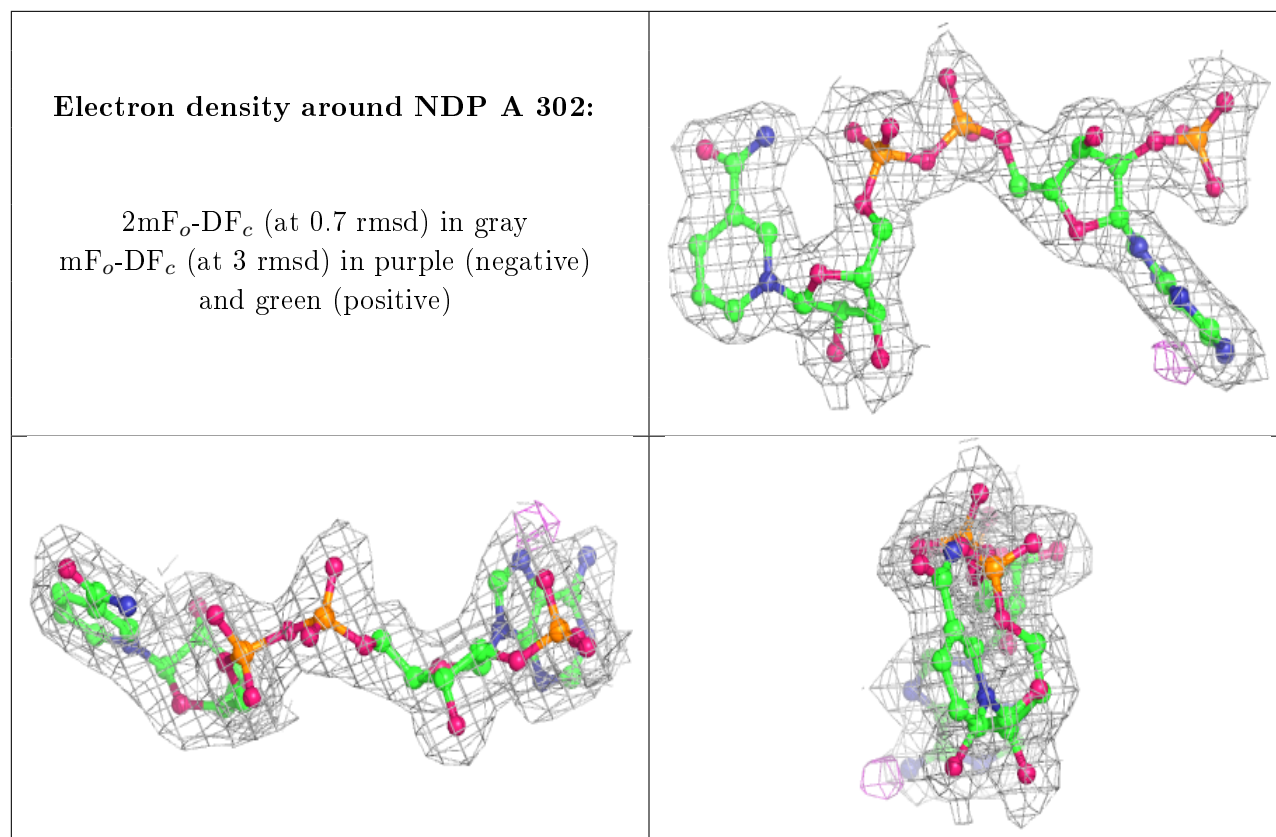
Electron density around NDP B 302:

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

**Electron density around NDP C 302:**

$2mF_o-DF_c$ (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.