



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:30 PM UTC

PDB ID : 6AVP / pdb_00006avp
Title : Staphylococcus aureus Type II pantothenate kinase in complex with ADP and pantothenate analog Phosphate-MeO-N5Pan
Authors : Chen, Y.; Antoshchenko, T.; Strauss, E.; Barnard, L.; Huang, Y.H.
Deposited on : 2017-09-04
Resolution : 2.30 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

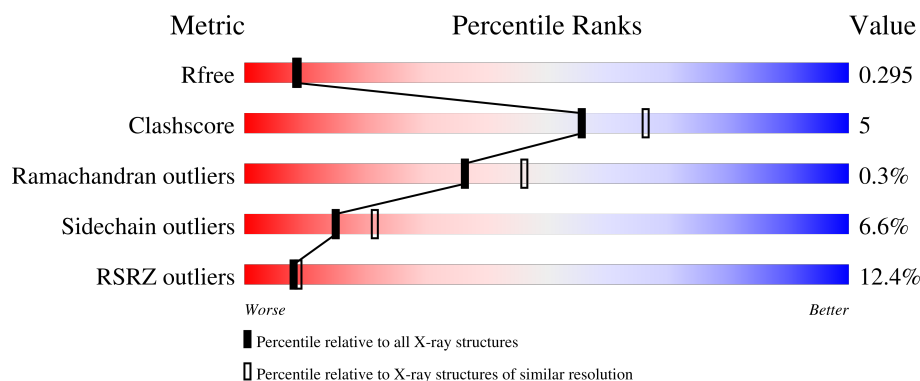
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	265	9% 87% 12%
1	B	265	7% 86% 12%
1	C	265	18% 85% 11%
1	D	265	15% 89% 8%

2 Entry composition [i](#)

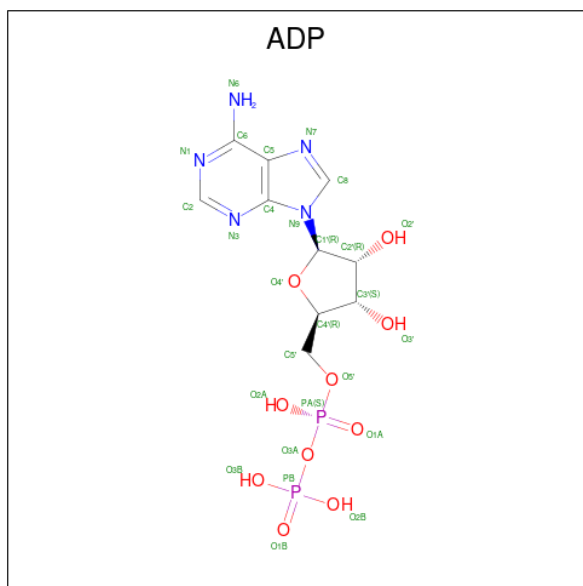
There are 5 unique types of molecules in this entry. The entry contains 8435 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Type II pantothenate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2033	1287	349	391	6			
1	B	265	Total	C	N	O	S	0	0	0
			2033	1287	349	391	6			
1	C	259	Total	C	N	O	S	0	0	0
			1982	1258	339	380	5			
1	D	259	Total	C	N	O	S	0	0	0
			1982	1258	339	380	5			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



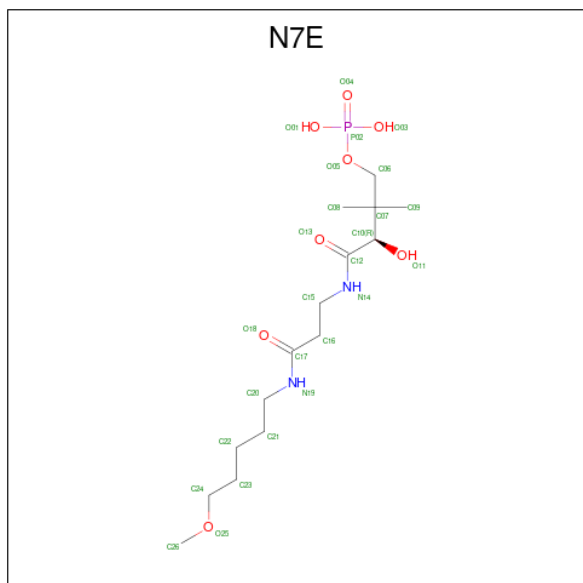
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is N 3 -[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(5-methoxy pentyl)-beta-alaninamide (CCD ID: N7E) (formula: C₁₅H₃₁N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			26	15	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			26	15	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			26	15	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			26	15	2	8	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Mg 1	0	0

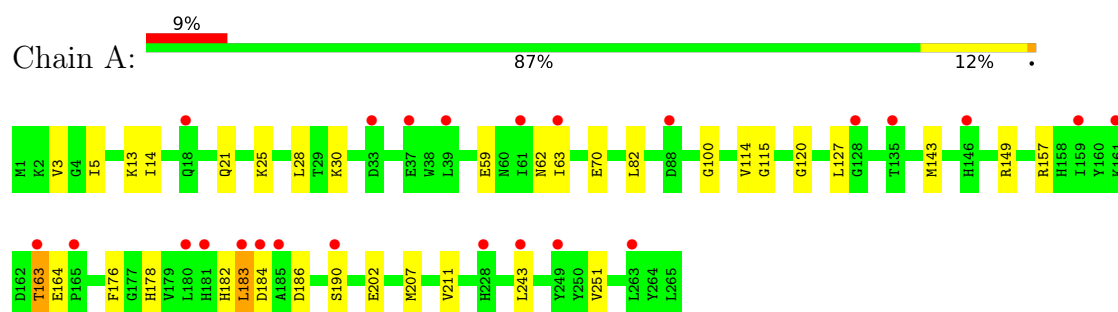
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total 47	O 47	0	0
5	B	46	Total 46	O 46	0	0
5	C	57	Total 57	O 57	0	0
5	D	39	Total 39	O 39	0	0

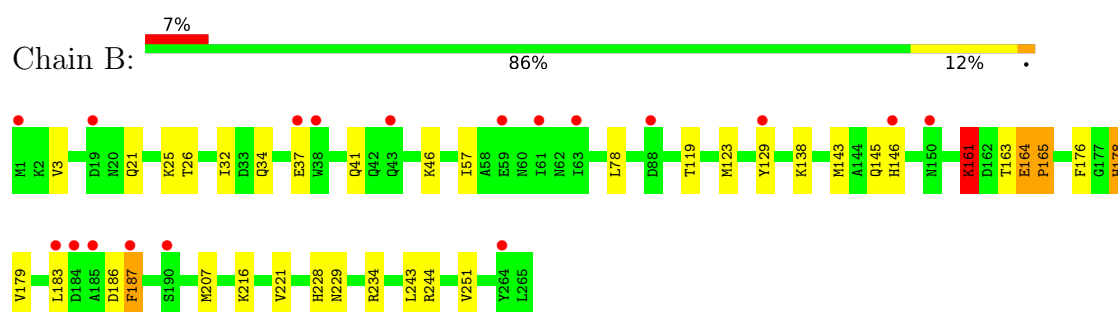
3 Residue-property plots [i](#)

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.

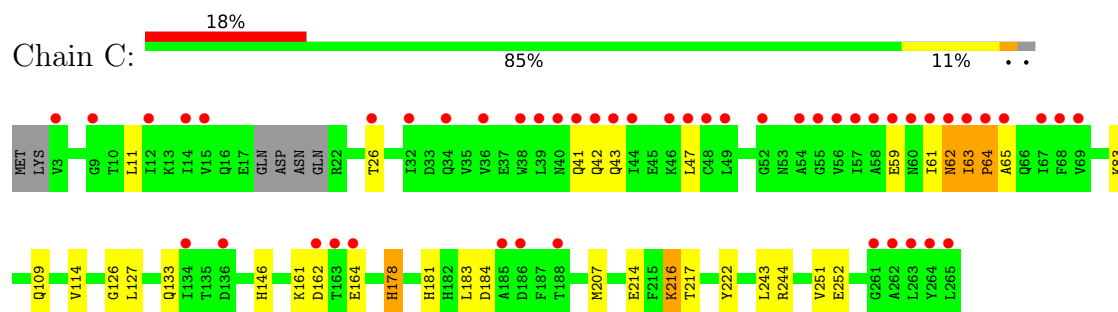
- Molecule 1: Type II pantothenate kinase



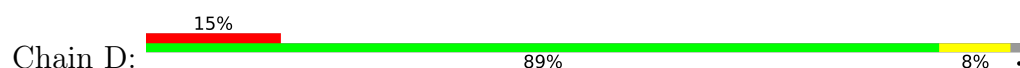
- Molecule 1: Type II pantothenate kinase

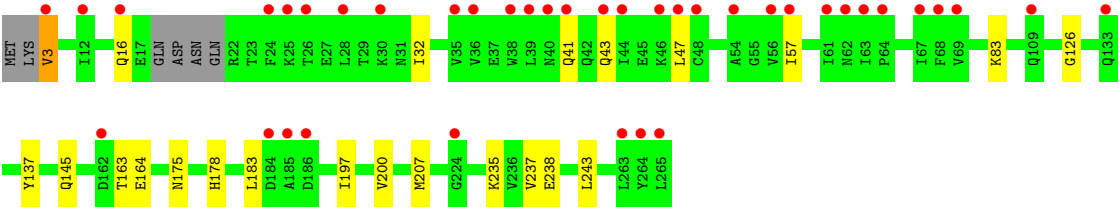


- Molecule 1: Type II pantothenate kinase



- Molecule 1: Type II pantothenate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.57Å 56.70Å 133.07Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	131.35 – 2.30 131.35 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (131.35-2.30) 99.4 (131.35-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.245 , 0.295 0.247 , 0.295	Depositor DCC
R_{free} test set	2410 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8435	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.71% 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: ADP, N7E, MG

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	0.69	0/2068	0.91	0/2801
1	B	0.79	2/2068 (0.1%)	0.97	2/2801 (0.1%)
1	C	0.78	2/2016 (0.1%)	0.97	5/2731 (0.2%)
1	D	0.68	2/2016 (0.1%)	0.92	2/2731 (0.1%)
All	All	0.74	6/8168 (0.1%)	0.94	9/11064 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	235	LYS	C-O	-5.73	1.17	1.24
1	C	217	THR	C-O	-5.70	1.16	1.24
1	D	237	VAL	C-O	-5.48	1.18	1.24
1	B	228	HIS	C-O	-5.47	1.17	1.23
1	B	165	PRO	CA-C	5.29	1.54	1.51
1	C	214	GLU	C-O	-5.15	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	GLU	CA-C-N	9.53	126.62	119.66
1	B	164	GLU	C-N-CA	9.53	126.62	119.66
1	C	183	LEU	N-CA-C	6.73	118.28	111.07
1	C	62	ASN	N-CA-C	6.45	119.27	111.40
1	C	63	ILE	CA-C-N	6.19	127.58	119.84
1	C	63	ILE	C-N-CA	6.19	127.58	119.84
1	D	145	GLN	N-CA-C	5.67	117.46	111.28
1	D	238	GLU	N-CA-C	5.25	116.69	111.07
1	C	216	LYS	N-CA-C	5.01	118.50	111.74

There are no chirality outliers.

There are no planarity outliers.

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	2033	0	2021	26	0
1	B	2033	0	2021	26	0
1	C	1982	0	1969	23	0
1	D	1982	0	1969	8	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	1	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	47	0	0	20	0
5	B	46	0	0	10	0
5	C	57	0	0	12	0
5	D	39	0	0	0	0
All	All	8435	0	8028	77	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 5.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD23	5:A:433:HOH:O	1.47	1.12
1:A:182:HIS:CD2	5:A:405:HOH:O	2.00	1.11
1:C:222:TYR:O	5:C:401:HOH:O	1.77	1.02
1:B:146:HIS:N	5:B:401:HOH:O	1.68	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLN:CA	5:B:401:HOH:O	2.15	0.94
1:C:63:ILE:CG1	1:C:64:PRO:HD2	1.98	0.94
1:C:63:ILE:HG13	1:C:64:PRO:HD2	1.49	0.93
1:B:207:MET:HE2	5:B:440:HOH:O	1.70	0.92
1:B:123:MET:HE2	1:D:175:ASN:HB2	1.56	0.87
1:C:164:GLU:OE1	5:C:402:HOH:O	1.94	0.85
1:B:145:GLN:HB2	5:B:401:HOH:O	1.77	0.84
1:B:145:GLN:N	5:B:401:HOH:O	2.13	0.81
1:C:252:GLU:OE2	5:C:403:HOH:O	1.98	0.80
1:C:164:GLU:CD	5:C:404:HOH:O	2.29	0.76
1:A:120:GLY:HA3	5:A:415:HOH:O	1.84	0.75
1:C:63:ILE:HG13	1:C:64:PRO:CD	2.16	0.75
1:A:114:VAL:C	5:A:403:HOH:O	2.33	0.70
1:B:163:THR:HG22	1:B:164:GLU:N	2.07	0.69
1:C:63:ILE:HG12	1:C:64:PRO:HD2	1.75	0.67
1:A:100:GLY:HA2	5:A:415:HOH:O	1.94	0.66
1:A:115:GLY:N	5:A:403:HOH:O	2.28	0.66
1:C:164:GLU:OE1	5:C:404:HOH:O	2.12	0.66
1:A:182:HIS:HD2	5:A:405:HOH:O	1.55	0.65
1:A:70:GLU:OE2	5:A:402:HOH:O	2.17	0.60
1:C:244:ARG:NH2	5:C:405:HOH:O	2.18	0.60
1:B:163:THR:CG2	1:B:164:GLU:N	2.65	0.59
1:B:145:GLN:CB	5:B:401:HOH:O	2.33	0.58
5:A:422:HOH:O	1:C:114:VAL:HA	2.03	0.58
1:C:164:GLU:HB3	5:C:404:HOH:O	2.04	0.56
1:C:178:HIS:HA	5:C:406:HOH:O	2.05	0.55
1:C:244:ARG:NH1	5:C:405:HOH:O	2.33	0.54
1:C:181:HIS:CD2	5:C:406:HOH:O	2.61	0.53
1:B:163:THR:O	1:B:165:PRO:HD3	2.09	0.53
1:A:100:GLY:N	5:A:401:HOH:O	1.88	0.52
1:A:207:MET:SD	1:C:207:MET:SD	3.08	0.51
1:B:145:GLN:HG2	5:B:430:HOH:O	2.11	0.51
1:B:129:TYR:C	1:B:129:TYR:CD1	2.87	0.51
1:C:146:HIS:HD2	5:C:449:HOH:O	1.94	0.50
1:A:5:ILE:HG12	1:A:14:ILE:HG12	1.93	0.49
1:A:157:ARG:NH1	5:A:404:HOH:O	2.42	0.49
1:A:30:LYS:HD3	5:A:425:HOH:O	2.12	0.48
1:B:119:THR:HA	1:B:123:MET:HE3	1.95	0.48
1:A:176:PHE:O	1:C:126:GLY:HA3	2.13	0.48
1:A:183:LEU:O	1:A:184:ASP:HB2	2.14	0.48
1:B:229:ASN:CG	5:B:402:HOH:O	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:CG1	1:C:64:PRO:CD	2.78	0.47
1:D:3:VAL:HG23	1:D:16:GLN:HG2	1.96	0.47
1:B:138:LYS:HG3	5:B:429:HOH:O	2.13	0.47
1:C:181:HIS:CG	5:C:406:HOH:O	2.68	0.47
1:D:137:TYR:CZ	2:D:301:ADP:C8	3.04	0.46
1:B:186:ASP:O	1:B:187:PHE:HB2	2.16	0.46
1:C:47:LEU:HD23	1:C:65:ALA:HB2	1.96	0.46
1:A:207:MET:HE2	5:A:439:HOH:O	2.15	0.46
1:D:32:ILE:HD11	1:D:57:ILE:HG13	1.98	0.45
1:B:207:MET:SD	1:D:207:MET:SD	3.15	0.45
1:A:100:GLY:CA	5:A:415:HOH:O	2.60	0.44
1:D:3:VAL:CG1	1:D:47:LEU:HD13	2.48	0.44
1:B:78:LEU:HD11	1:B:221:VAL:HG11	2.00	0.43
1:B:32:ILE:HD11	1:B:57:ILE:HG13	2.00	0.43
1:A:62:ASN:C	1:A:63:ILE:HG13	2.44	0.43
1:B:119:THR:HG22	1:B:123:MET:HE1	2.00	0.43
1:B:178:HIS:O	1:B:179:VAL:C	2.62	0.43
1:B:145:GLN:CG	5:B:430:HOH:O	2.67	0.42
1:A:190:SER:HB2	5:A:434:HOH:O	2.18	0.42
1:C:61:ILE:CG2	1:C:62:ASN:N	2.82	0.42
1:B:161:LYS:HD2	1:B:161:LYS:HA	1.72	0.42
1:A:163:THR:HG21	5:A:442:HOH:O	2.20	0.42
1:D:197:ILE:HA	1:D:200:VAL:HG12	2.02	0.42
1:B:186:ASP:OD1	1:B:186:ASP:N	2.50	0.41
1:A:100:GLY:C	5:A:415:HOH:O	2.63	0.41
1:B:176:PHE:O	1:D:126:GLY:HA3	2.20	0.41
1:A:30:LYS:HE3	5:A:414:HOH:O	2.21	0.41
1:A:120:GLY:CA	5:A:415:HOH:O	2.58	0.41
1:B:164:GLU:HA	1:B:165:PRO:HD2	1.75	0.41
1:A:127:LEU:HD11	1:C:127:LEU:HD11	2.03	0.40
1:A:143:MET:HG2	5:A:434:HOH:O	2.21	0.40
1:A:149:ARG:NH2	1:A:202:GLU:OE2	2.51	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	263/265 (99%)	250 (95%)	13 (5%)	0	100	100
1	B	263/265 (99%)	248 (94%)	13 (5%)	2 (1%)	16	20
1	C	255/265 (96%)	248 (97%)	6 (2%)	1 (0%)	30	38
1	D	255/265 (96%)	245 (96%)	10 (4%)	0	100	100
All	All	1036/1060 (98%)	991 (96%)	42 (4%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	PHE
1	B	161	LYS
1	C	64	PRO

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	215/215 (100%)	201 (94%)	14 (6%)	15	22
1	B	215/215 (100%)	198 (92%)	17 (8%)	11	15
1	C	209/215 (97%)	193 (92%)	16 (8%)	12	16
1	D	209/215 (97%)	200 (96%)	9 (4%)	26	39
All	All	848/860 (99%)	792 (93%)	56 (7%)	15	21

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	13	LYS
1	A	21	GLN

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Mol	Chain	Res	Type
1	A	25	LYS
1	A	28	LEU
1	A	59	GLU
1	A	163	THR
1	A	164	GLU
1	A	178	HIS
1	A	183	LEU
1	A	186	ASP
1	A	211	VAL
1	A	243	LEU
1	A	251	VAL
1	B	3	VAL
1	B	21	GLN
1	B	25	LYS
1	B	26	THR
1	B	34	GLN
1	B	37	GLU
1	B	41	GLN
1	B	46	LYS
1	B	143	MET
1	B	161	LYS
1	B	178	HIS
1	B	183	LEU
1	B	216	LYS
1	B	234	ARG
1	B	243	LEU
1	B	244	ARG
1	B	251	VAL
1	C	11	LEU
1	C	26	THR
1	C	41	GLN
1	C	42	GLN
1	C	43	GLN
1	C	59	GLU
1	C	83	LYS
1	C	109	GLN
1	C	133	GLN
1	C	161	LYS
1	C	162	ASP
1	C	178	HIS
1	C	184	ASP
1	C	216	LYS

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Mol	Chain	Res	Type
1	C	243	LEU
1	C	251	VAL
1	D	3	VAL
1	D	41	GLN
1	D	43	GLN
1	D	83	LYS
1	D	163	THR
1	D	164	GLU
1	D	178	HIS
1	D	183	LEU
1	D	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	42	GLN
1	A	53	ASN
1	A	125	GLN
1	A	178	HIS
1	A	182	HIS
1	A	219	ASN
1	B	42	GLN
1	B	53	ASN
1	B	76	GLN
1	B	139	GLN
1	B	178	HIS
1	B	182	HIS
1	B	228	HIS
1	B	253	ASN
1	C	133	GLN
1	C	146	HIS
1	C	181	HIS
1	D	76	GLN
1	D	146	HIS
1	D	178	HIS

5.3.3 RNA ⓘ

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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	N7E	C	302	4	23,25,25	0.86	0	30,33,33	1.69	4 (13%)
2	ADP	C	301	4	28,29,29	1.58	5 (17%)	43,45,45	2.02	7 (16%)
3	N7E	A	302	4	23,25,25	0.87	1 (4%)	30,33,33	1.69	7 (23%)
2	ADP	A	301	4	28,29,29	1.42	3 (10%)	43,45,45	1.94	9 (20%)
2	ADP	B	301	4	28,29,29	1.43	5 (17%)	43,45,45	1.98	9 (20%)
3	N7E	D	302	4	23,25,25	0.91	1 (4%)	30,33,33	1.57	4 (13%)
3	N7E	B	302	4	23,25,25	1.00	1 (4%)	30,33,33	1.63	7 (23%)
2	ADP	D	301	4	28,29,29	1.75	6 (21%)	43,45,45	1.95	9 (20%)

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	N7E	C	302	4	-	3/31/31/31	-
2	ADP	C	301	4	-	2/16/32/32	0/3/3/3
3	N7E	A	302	4	-	1/31/31/31	-
2	ADP	A	301	4	-	8/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	301	4	-	3/16/32/32	0/3/3/3
3	N7E	D	302	4	-	2/31/31/31	-
3	N7E	B	302	4	-	2/31/31/31	-
2	ADP	D	301	4	-	3/16/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	ADP	C5-C4	5.11	1.48	1.39
2	C	301	ADP	C5-C4	4.93	1.47	1.39
2	D	301	ADP	PA-O3A	4.62	1.64	1.59
2	B	301	ADP	C5-C4	4.44	1.47	1.39
2	A	301	ADP	C5-C4	4.34	1.46	1.39
2	C	301	ADP	C5-N7	-3.15	1.33	1.39
2	B	301	ADP	C5-N7	-3.04	1.33	1.39
2	D	301	ADP	C5-C6	2.85	1.48	1.41
2	A	301	ADP	C5-N7	-2.83	1.33	1.39
2	D	301	ADP	C5-N7	-2.82	1.33	1.39
2	C	301	ADP	C5-C6	2.70	1.48	1.41
2	A	301	ADP	C5-C6	2.63	1.48	1.41
2	C	301	ADP	C8-N7	2.57	1.36	1.31
2	C	301	ADP	PA-O3A	2.54	1.62	1.59
3	B	302	N7E	C06-C07	2.50	1.56	1.52
2	B	301	ADP	C5-C6	2.45	1.47	1.41
2	B	301	ADP	PA-O3A	2.29	1.62	1.59
2	D	301	ADP	C8-N7	2.29	1.36	1.31
3	A	302	N7E	C06-C07	2.26	1.56	1.52
2	D	301	ADP	C8-N9	-2.05	1.34	1.37
2	B	301	ADP	C8-N7	2.03	1.35	1.31
3	D	302	N7E	P02-O03	-2.01	1.47	1.54

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	ADP	C5-C4-N3	-7.25	116.73	126.72
2	D	301	ADP	C5-C4-N3	-6.82	117.32	126.72
2	B	301	ADP	C5-C4-N3	-6.63	117.59	126.72
2	A	301	ADP	C5-C4-N3	-6.11	118.31	126.72
2	D	301	ADP	N3-C4-N9	5.47	136.47	127.17
3	D	302	N7E	O03-P02-O05	-5.45	92.45	106.67
2	B	301	ADP	N3-C4-N9	5.32	136.21	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	ADP	N3-C4-N9	5.28	136.15	127.17
2	A	301	ADP	N3-C4-N9	4.88	135.47	127.17
3	C	302	N7E	O03-P02-O05	-4.73	94.35	106.67
2	C	301	ADP	C2-N3-C4	4.48	122.76	111.83
3	C	302	N7E	O01-P02-O05	-4.34	95.35	106.67
2	A	301	ADP	C2-N3-C4	4.32	122.39	111.83
2	A	301	ADP	N3-C2-N1	-4.21	122.21	128.58
2	B	301	ADP	C2-N3-C4	4.13	121.91	111.83
2	D	301	ADP	C2-N3-C4	4.08	121.80	111.83
3	A	302	N7E	O03-P02-O05	-3.93	96.43	106.67
3	A	302	N7E	C15-C16-C17	-3.70	106.22	112.39
3	B	302	N7E	O05-P02-O04	-3.67	96.52	106.44
2	D	301	ADP	C4-C5-N7	-3.66	106.40	110.58
2	B	301	ADP	N3-C2-N1	-3.62	123.10	128.58
2	B	301	ADP	C4-C5-N7	-3.47	106.61	110.58
2	C	301	ADP	C4-C5-N7	-3.40	106.70	110.58
2	C	301	ADP	N3-C2-N1	-3.33	123.55	128.58
3	B	302	N7E	C15-C16-C17	-3.29	106.92	112.39
2	A	301	ADP	C4-C5-N7	-3.25	106.87	110.58
3	B	302	N7E	O01-P02-O05	-3.24	98.22	106.67
3	B	302	N7E	O03-P02-O05	-3.14	98.48	106.67
3	C	302	N7E	O03-P02-O01	3.11	119.48	107.80
3	A	302	N7E	O03-P02-O01	3.11	119.46	107.80
3	D	302	N7E	O03-P02-O01	3.06	119.29	107.80
2	D	301	ADP	N3-C2-N1	-3.05	123.96	128.58
3	A	302	N7E	O05-P02-O04	-2.90	98.60	106.44
2	B	301	ADP	C5-N7-C8	2.88	107.98	103.45
3	A	302	N7E	O01-P02-O05	-2.80	99.37	106.67
3	B	302	N7E	O03-P02-O01	2.75	118.10	107.80
3	D	302	N7E	O01-P02-O05	-2.67	99.71	106.67
2	A	301	ADP	C5-N7-C8	2.64	107.60	103.45
2	D	301	ADP	C5-N7-C8	2.64	107.60	103.45
3	B	302	N7E	O11-C10-C07	-2.52	104.34	110.18
3	C	302	N7E	C23-C22-C21	-2.48	101.82	114.37
2	C	301	ADP	C5-N7-C8	2.43	107.28	103.45
2	D	301	ADP	O3B-PB-O2B	2.43	116.90	107.80
2	B	301	ADP	O3B-PB-O2B	2.37	116.67	107.80
3	B	302	N7E	O01-P02-O04	2.33	119.92	110.83
2	A	301	ADP	C2-N1-C6	2.28	122.47	118.73
2	D	301	ADP	C1'-N9-C8	-2.28	122.04	127.09
2	D	301	ADP	C4-N9-C8	2.24	108.09	105.74
2	A	301	ADP	C4-N9-C8	2.23	108.08	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ADP	C1'-N9-C8	-2.23	122.15	127.09
2	B	301	ADP	C4-N9-C8	2.19	108.04	105.74
3	A	302	N7E	C20-N19-C17	-2.12	118.88	122.82
3	D	302	N7E	O05-P02-O04	-2.10	100.77	106.44
2	A	301	ADP	C1'-N9-C8	-2.07	122.49	127.09
2	C	301	ADP	O4'-C1'-N9	2.05	112.03	108.09
3	A	302	N7E	O01-P02-O04	2.01	118.68	110.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

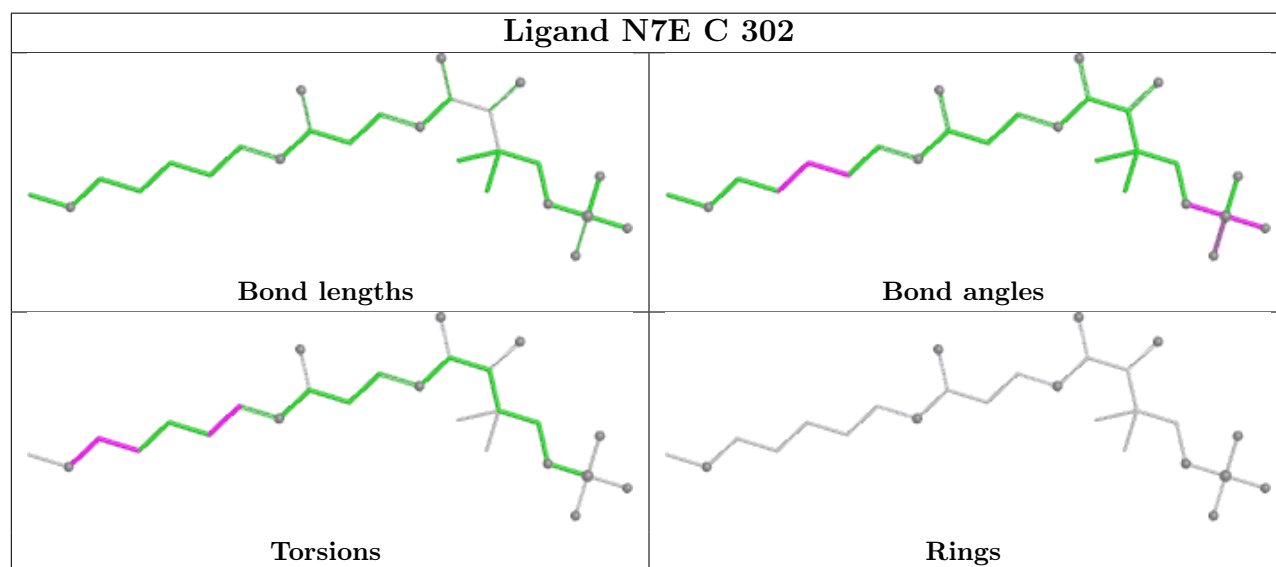
Mol	Chain	Res	Type	Atoms
2	A	301	ADP	C5'-O5'-PA-O1A
2	A	301	ADP	C5'-O5'-PA-O2A
2	C	301	ADP	C2'-C1'-N9-C4
3	A	302	N7E	N19-C20-C21-C22
2	C	301	ADP	C2'-C1'-N9-C8
3	B	302	N7E	C22-C23-C24-O25
3	C	302	N7E	N19-C20-C21-C22
3	C	302	N7E	C22-C23-C24-O25
2	B	301	ADP	C2'-C1'-N9-C8
2	B	301	ADP	C2'-C1'-N9-C4
2	A	301	ADP	O4'-C4'-C5'-O5'
2	A	301	ADP	C2'-C1'-N9-C8
2	A	301	ADP	C3'-C4'-C5'-O5'
2	A	301	ADP	C2'-C1'-N9-C4
2	D	301	ADP	C2'-C1'-N9-C4
3	B	302	N7E	C20-C21-C22-C23
2	D	301	ADP	C2'-C1'-N9-C8
2	A	301	ADP	C5'-O5'-PA-O3A
3	D	302	N7E	C20-C21-C22-C23
2	A	301	ADP	PB-O3A-PA-O2A
2	B	301	ADP	PB-O3A-PA-O1A
3	D	302	N7E	C22-C23-C24-O25
3	C	302	N7E	C23-C24-O25-C26
2	D	301	ADP	PB-O3A-PA-O2A

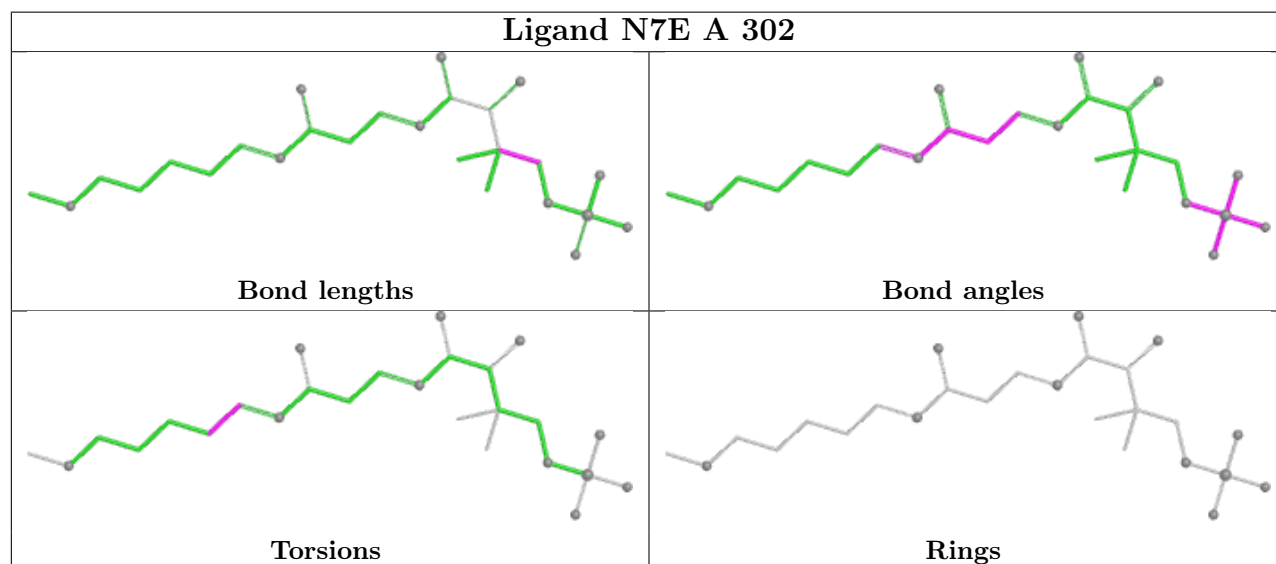
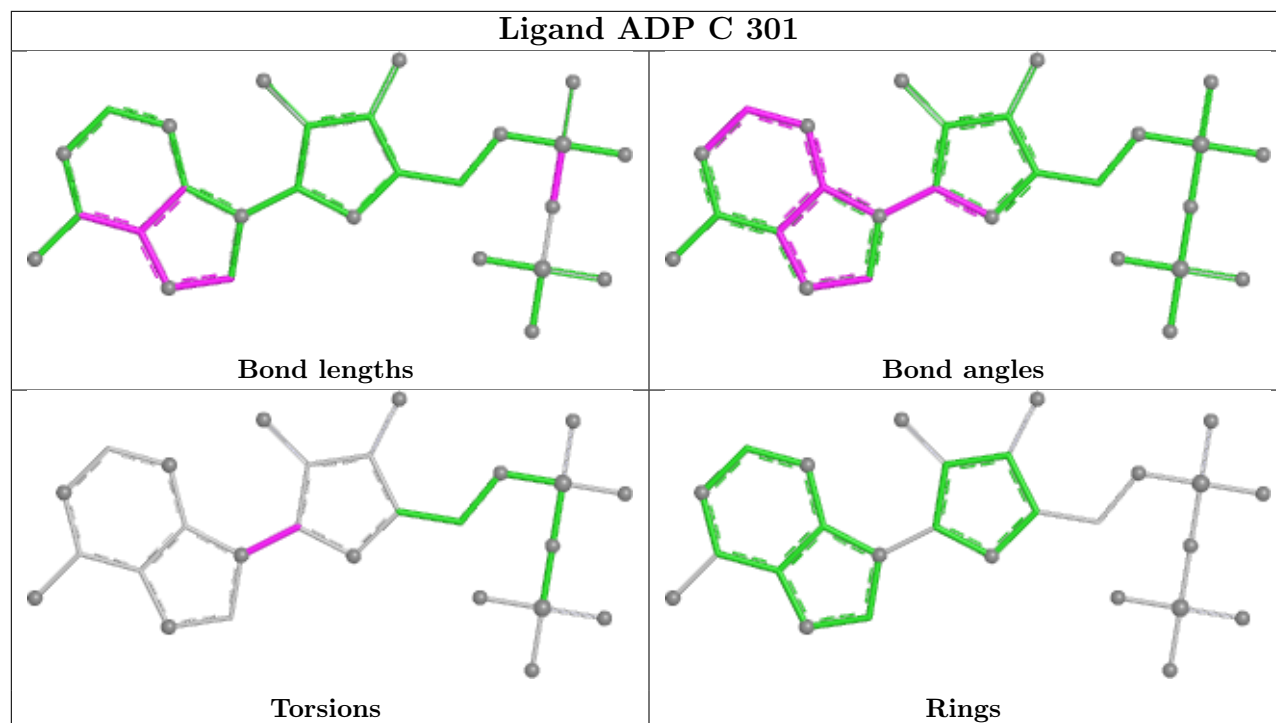
There are no ring outliers.

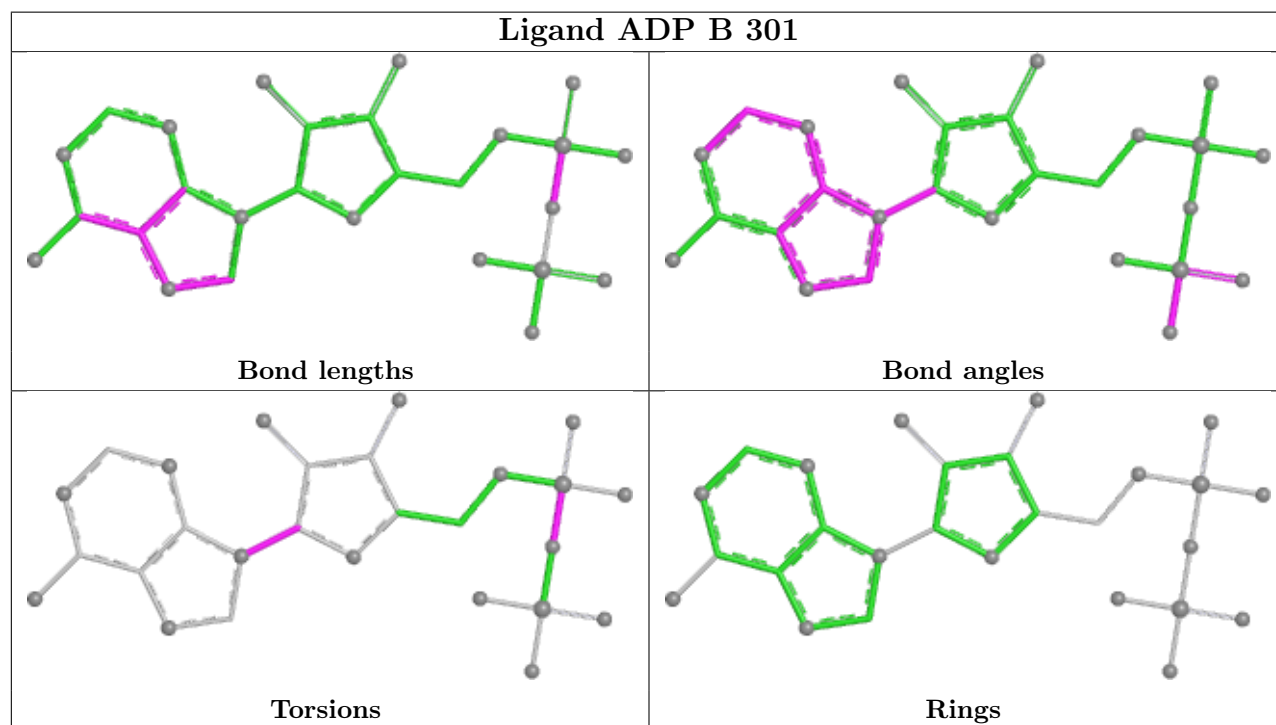
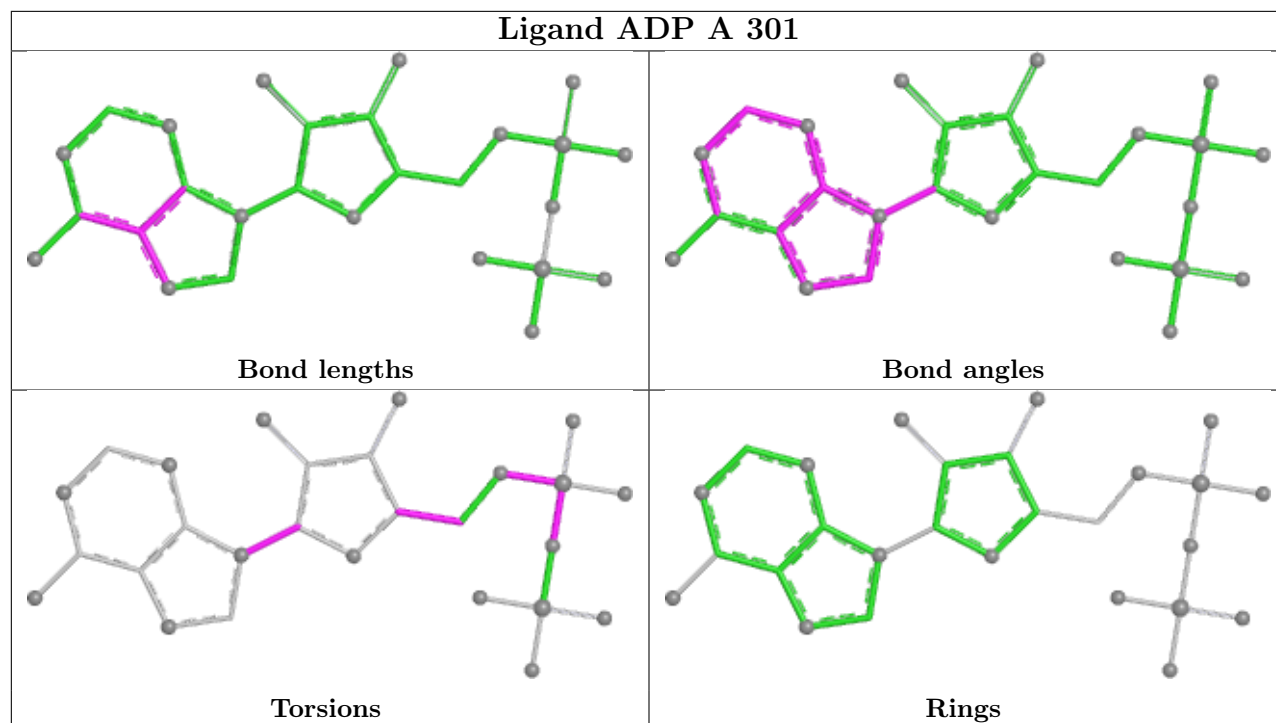
1 monomer is involved in 1 short contact:

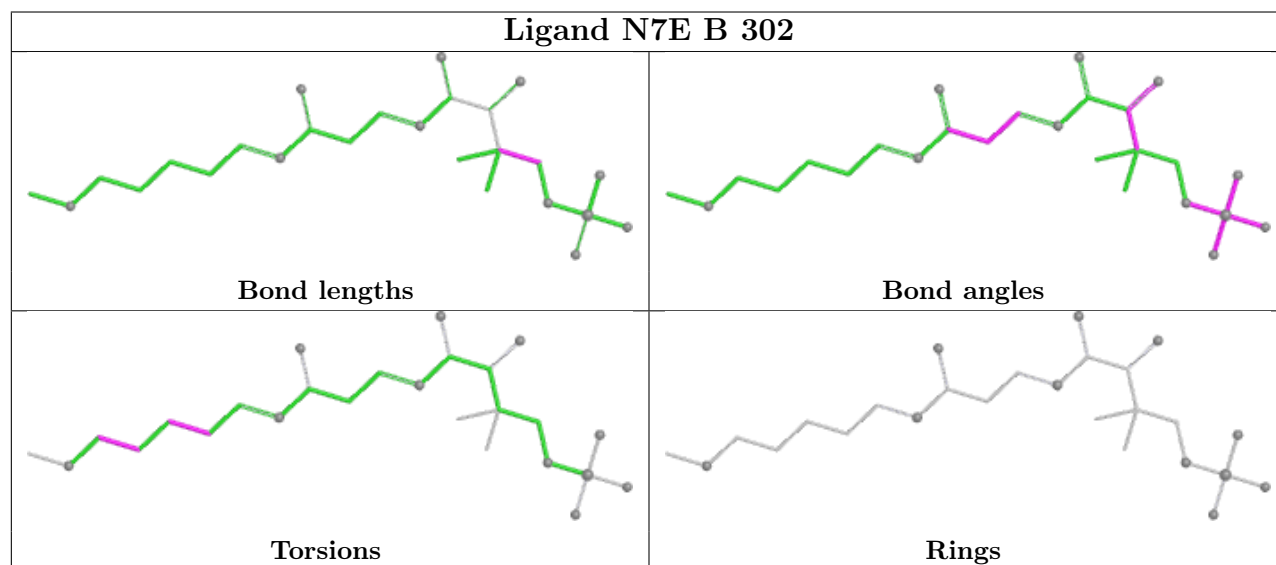
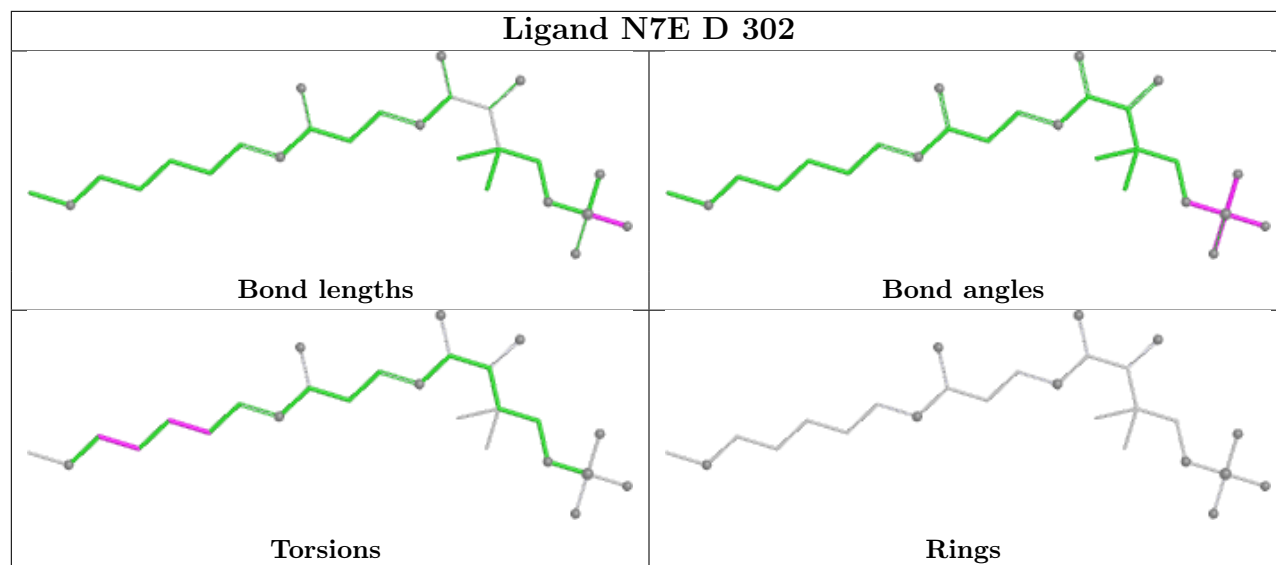
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	ADP	1	0

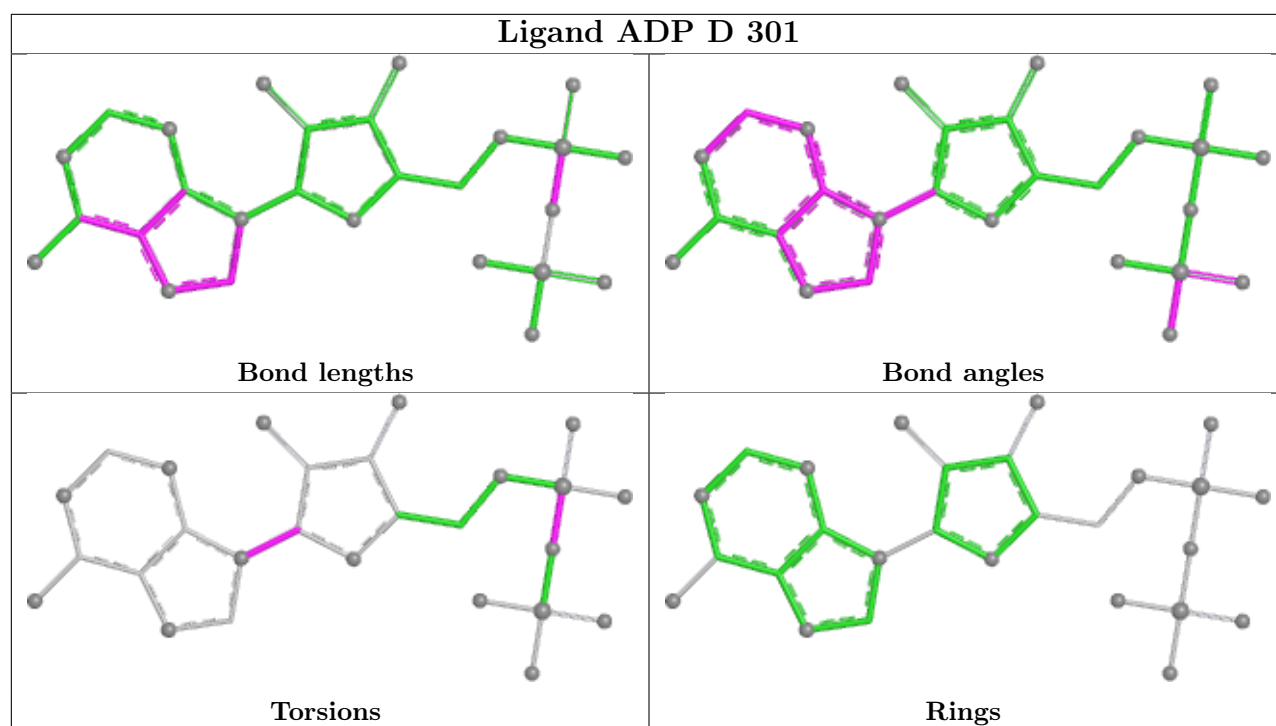
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	265/265 (100%)	0.92	24 (9%) 15 16	14, 34, 59, 89	0
1	B	265/265 (100%)	0.91	18 (6%) 23 25	20, 38, 66, 92	0
1	C	259/265 (97%)	1.21	49 (18%) 3 4	13, 32, 84, 111	0
1	D	259/265 (97%)	1.13	39 (15%) 5 6	18, 38, 88, 100	0
All	All	1048/1060 (98%)	1.04	130 (12%) 8 9	13, 35, 77, 111	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	VAL	5.5
1	A	184	ASP	5.5
1	C	63	ILE	5.3
1	D	264	TYR	4.7
1	C	57	ILE	4.6
1	A	185	ALA	4.5
1	B	61	ILE	4.5
1	C	61	ILE	4.4
1	B	264	TYR	4.3
1	C	65	ALA	4.3
1	C	264	TYR	4.2
1	C	41	GLN	4.2
1	C	58	ALA	4.2
1	C	64	PRO	4.0
1	C	47	LEU	3.9
1	C	62	ASN	3.9
1	A	181	HIS	3.9
1	C	60	ASN	3.8
1	A	183	LEU	3.5
1	C	265	LEU	3.5
1	D	63	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	162	ASP	3.4
1	A	63	ILE	3.3
1	C	67	ILE	3.3
1	C	163	THR	3.3
1	D	56	VAL	3.3
1	C	186	ASP	3.2
1	C	164	GLU	3.2
1	D	61	ILE	3.2
1	A	163	THR	3.2
1	D	185	ALA	3.1
1	D	16	GLN	3.1
1	C	40	ASN	3.1
1	D	186	ASP	3.1
1	D	44	ILE	3.0
1	C	42	GLN	3.0
1	B	37	GLU	3.0
1	C	55	GLY	3.0
1	C	162	ASP	3.0
1	C	12	ILE	2.9
1	D	26	THR	2.9
1	D	38	TRP	2.9
1	A	161	LYS	2.9
1	C	3	VAL	2.9
1	D	3	VAL	2.9
1	D	57	ILE	2.9
1	D	67	ILE	2.9
1	C	68	PHE	2.8
1	D	43	GLN	2.8
1	B	187	PHE	2.8
1	D	36	VAL	2.8
1	C	44	ILE	2.8
1	B	146	HIS	2.7
1	C	14	ILE	2.7
1	A	190	SER	2.7
1	C	263	LEU	2.7
1	C	36	VAL	2.7
1	D	64	PRO	2.7
1	D	47	LEU	2.7
1	D	69	VAL	2.6
1	C	32	ILE	2.6
1	D	62	ASN	2.6
1	B	129	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	35	VAL	2.6
1	A	228	HIS	2.6
1	A	180	LEU	2.6
1	D	25	LYS	2.6
1	D	41	GLN	2.5
1	A	37	GLU	2.5
1	D	39	LEU	2.5
1	B	185	ALA	2.5
1	C	9	GLY	2.5
1	D	263	LEU	2.5
1	A	263	LEU	2.5
1	C	262	ALA	2.5
1	C	48	CYS	2.5
1	D	48	CYS	2.5
1	D	133	GLN	2.5
1	D	28	LEU	2.5
1	D	224	GLY	2.5
1	B	59	GLU	2.4
1	B	19	ASP	2.4
1	A	18	GLN	2.4
1	D	40	ASN	2.4
1	A	165	PRO	2.4
1	C	69	VAL	2.4
1	C	39	LEU	2.4
1	C	49	LEU	2.4
1	D	24	PHE	2.3
1	C	136	ASP	2.3
1	C	185	ALA	2.3
1	A	39	LEU	2.3
1	B	38	TRP	2.3
1	D	54	ALA	2.3
1	C	26	THR	2.3
1	A	61	ILE	2.3
1	C	46	LYS	2.3
1	C	15	VAL	2.3
1	A	88	ASP	2.2
1	B	88	ASP	2.2
1	C	34	GLN	2.2
1	C	188	THR	2.2
1	B	63	ILE	2.2
1	B	43	GLN	2.2
1	D	12	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	2.2
1	C	261	GLY	2.2
1	D	265	LEU	2.2
1	D	30	LYS	2.2
1	A	159	ILE	2.1
1	D	184	ASP	2.1
1	D	68	PHE	2.1
1	C	54	ALA	2.1
1	B	183	LEU	2.1
1	B	190	SER	2.1
1	A	128	GLY	2.1
1	A	135	THR	2.1
1	C	59	GLU	2.1
1	A	146	HIS	2.1
1	A	243	LEU	2.1
1	C	43	GLN	2.1
1	C	134	ILE	2.1
1	D	109	GLN	2.1
1	A	249	TYR	2.1
1	C	52	GLY	2.1
1	C	38	TRP	2.1
1	A	33	ASP	2.0
1	B	150	ASN	2.0
1	B	184	ASP	2.0
1	D	46	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

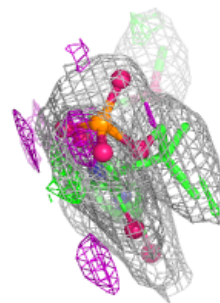
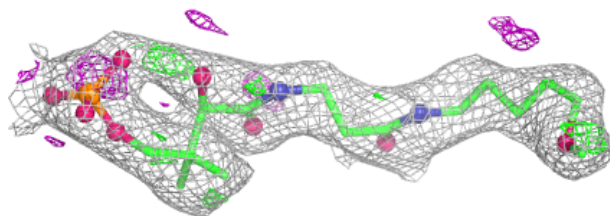
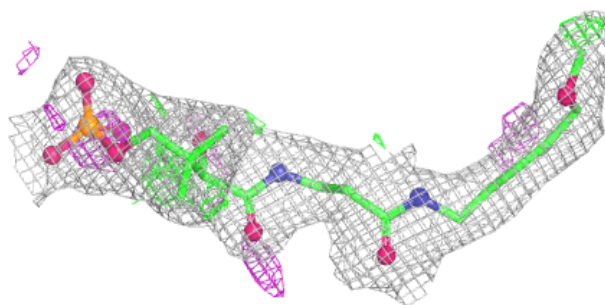
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	N7E	C	302	26/26	0.85	0.13	24,26,35,36	0
3	N7E	D	302	26/26	0.88	0.12	34,40,50,53	0
4	MG	B	303	1/1	0.90	0.06	40,40,40,40	0
2	ADP	D	301	27/27	0.92	0.09	24,26,33,33	0
4	MG	A	303	1/1	0.92	0.08	34,34,34,34	0
2	ADP	C	301	27/27	0.92	0.09	23,25,28,28	0
3	N7E	A	302	26/26	0.93	0.09	16,18,20,22	0
3	N7E	B	302	26/26	0.93	0.10	21,23,27,27	0
2	ADP	B	301	27/27	0.94	0.08	25,26,28,30	0
4	MG	D	303	1/1	0.94	0.04	39,39,39,39	0
2	ADP	A	301	27/27	0.95	0.08	19,22,26,27	0
4	MG	C	303	1/1	0.97	0.05	31,31,31,31	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.

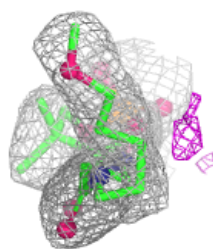
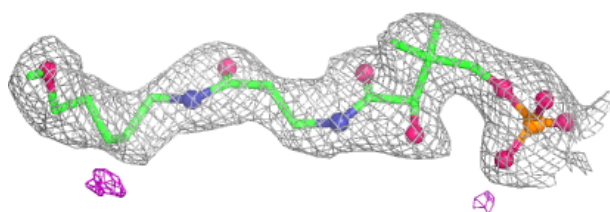
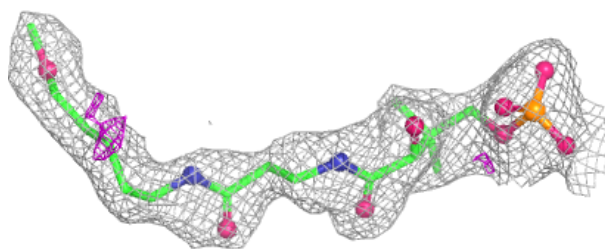
Electron density around N7E C 302:

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

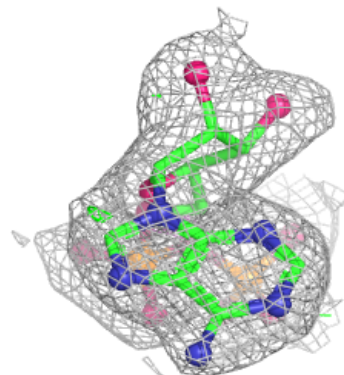
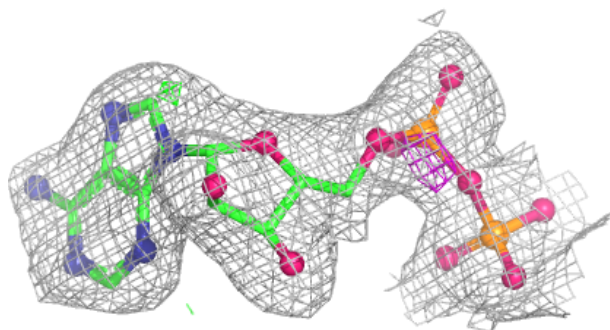
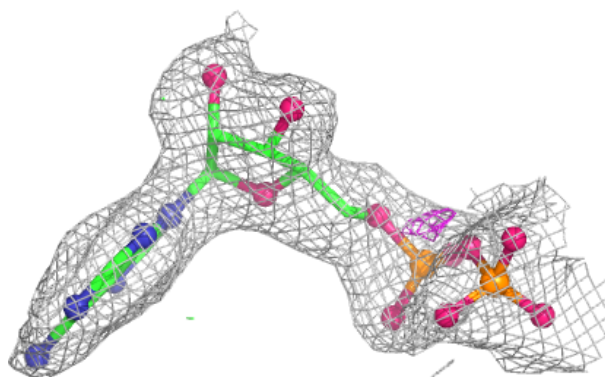


Electron density around N7E D 302:

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

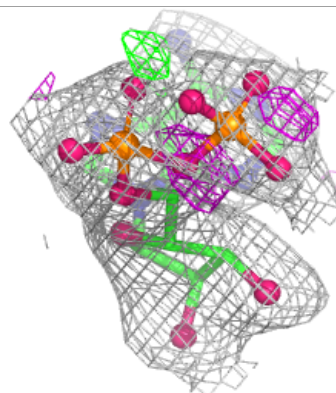
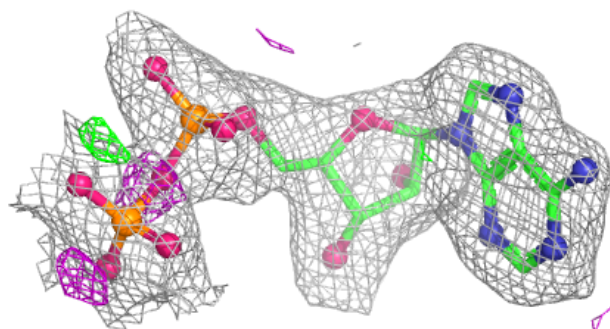
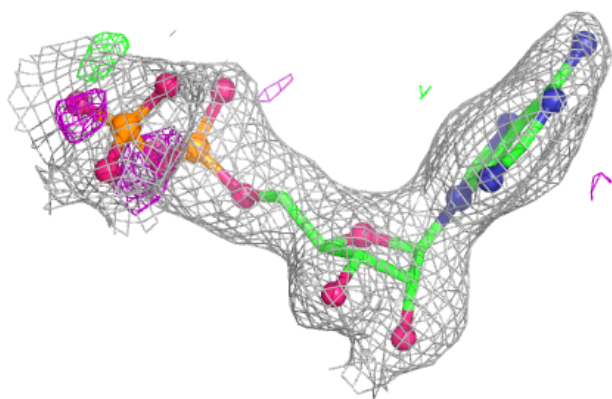
**Electron density around ADP D 301:**

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

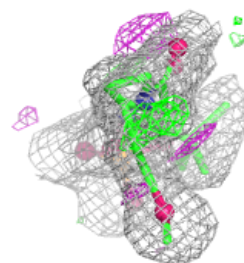
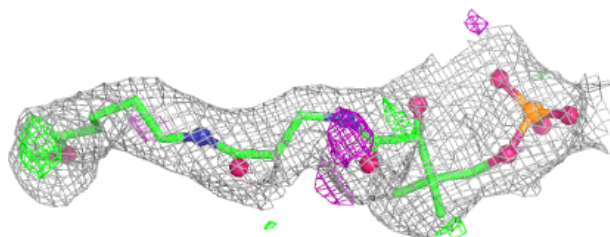
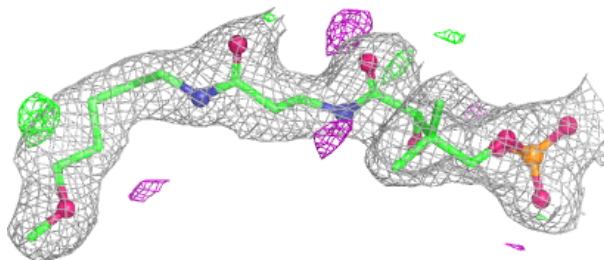


Electron density around ADP C 301:

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

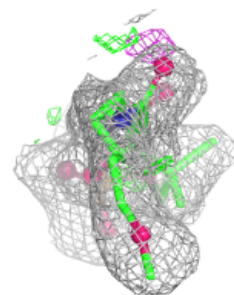
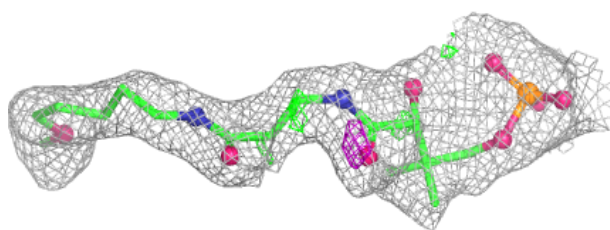
**Electron density around N7E A 302:**

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

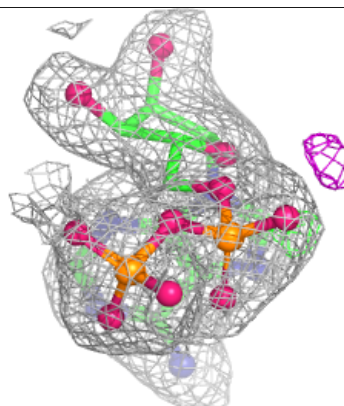
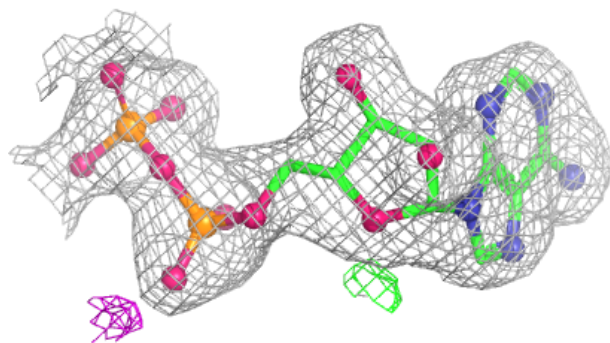
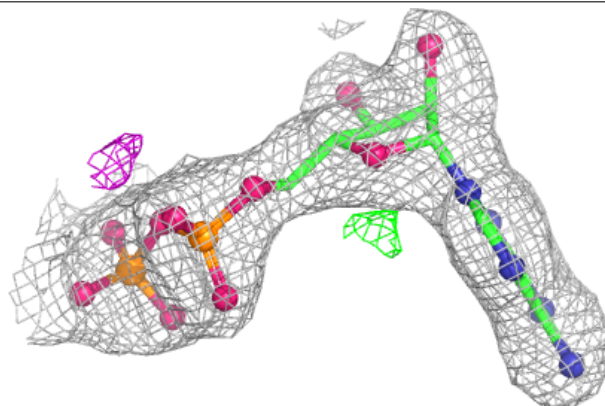


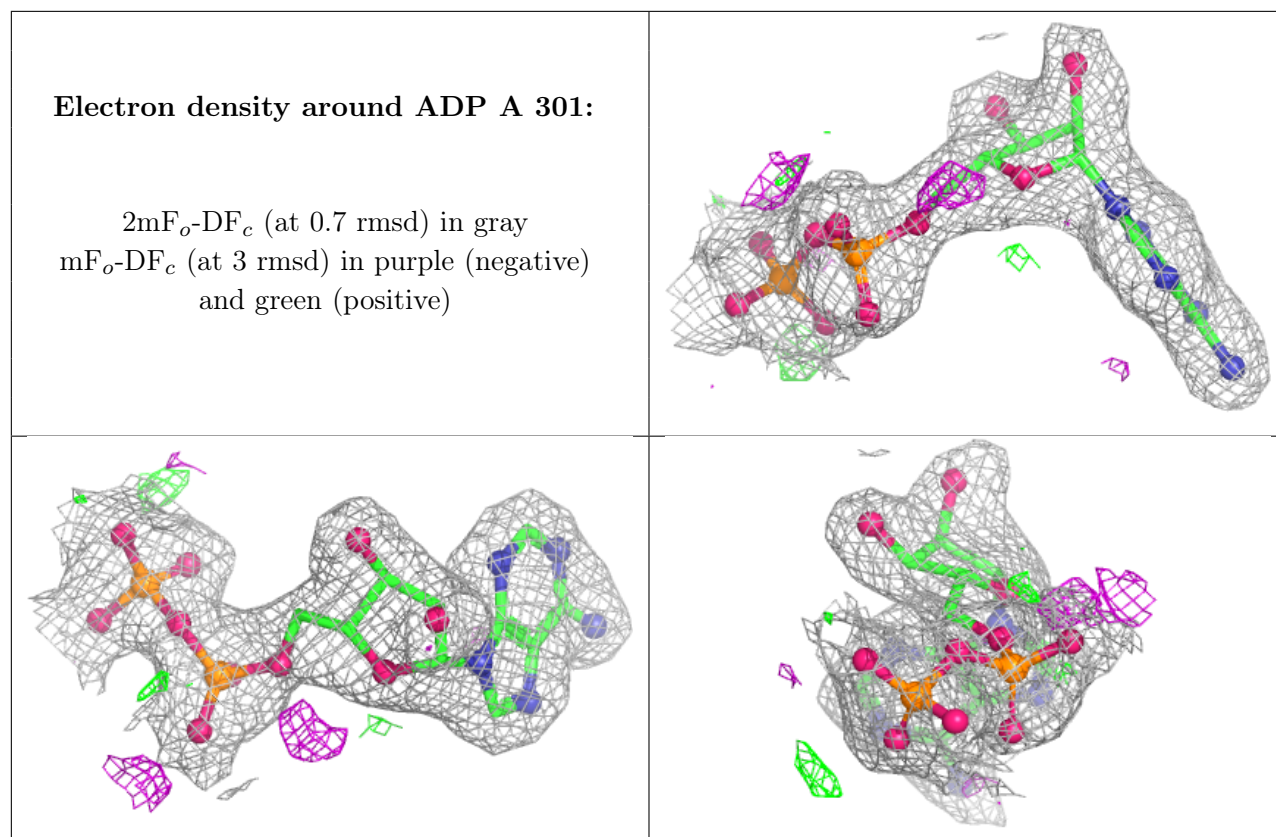
Electron density around N7E B 302:

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

**Electron density around ADP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.