



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:02 pm BST

PDB ID : 4NAT
Title : Inhibitors of 4-Phosphopanthetheine Adenylyltransferase
Authors : Lahiri, S.D.
Deposited on : 2013-10-22
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

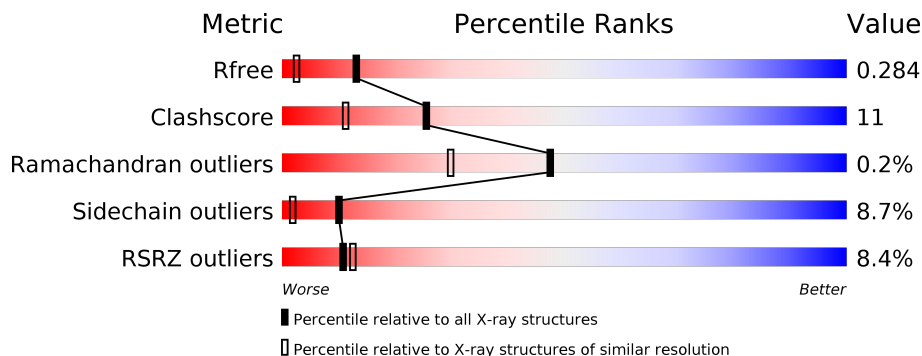
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	160	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 72% 20% . . .</p>
1	B	160	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 76% 15% 7% .</p>
1	C	160	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">11% 75% 20% . .</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2W5	A	201	X	-	-	-
4	ADP	B	203	-	-	-	X

2 Entry composition [i](#)

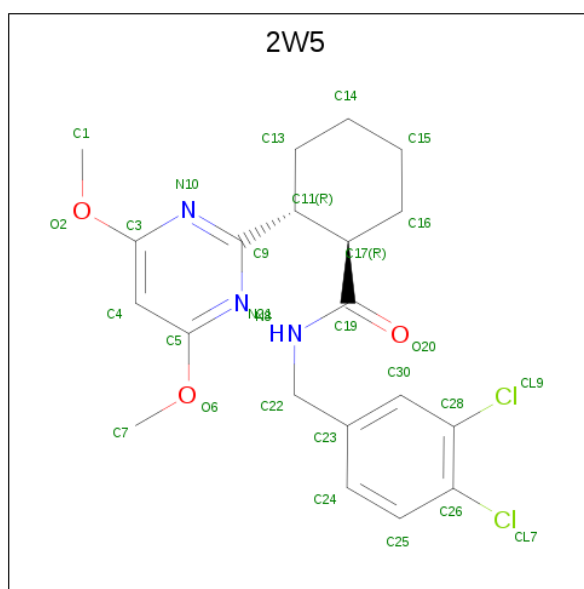
There are 5 unique types of molecules in this entry. The entry contains 4060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphopantetheine adenylyltransferase.

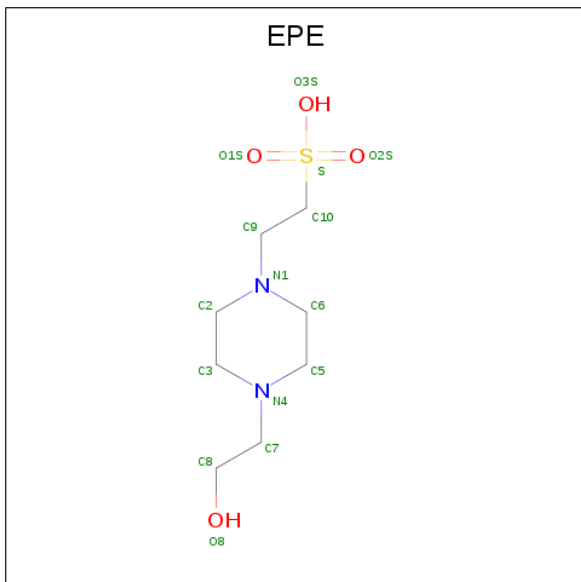
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	Total	C	N	O	S	0	1	0
			1235	791	203	234	7			
1	B	156	Total	C	N	O	S	0	1	0
			1261	807	207	240	7			
1	C	155	Total	C	N	O	S	0	1	0
			1252	802	206	236	8			

- Molecule 2 is (1R,2R)-N-(3,4-dichlorobenzyl)-2-(4,6-dimethoxypyrimidin-2-yl)cyclohexanecarboxamide (three-letter code: 2W5) (formula: C₂₀H₂₃Cl₂N₃O₃).



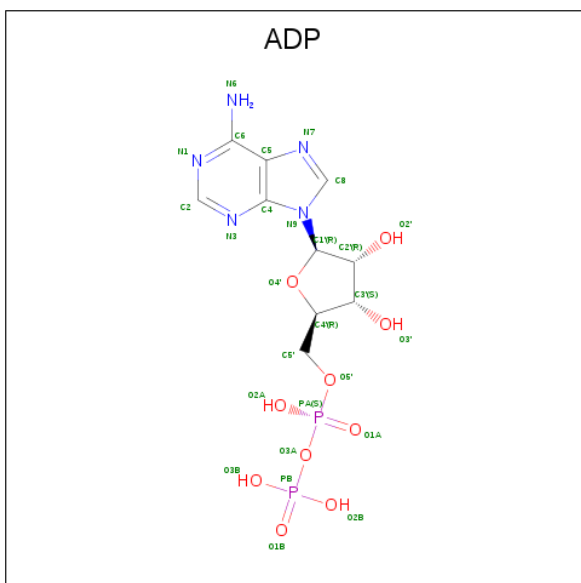
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	Total	C	Cl	N	O	0	0
			28	20	2	3	3		
2	B	1	Total	C	Cl	N	O	0	0
			28	20	2	3	3		
2	C	1	Total	C	Cl	N	O	0	0
			28	20	2	3	3		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	40	Total	O	0	0
			40	40		
5	C	42	Total	O	0	0
			42	42		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.16Å 127.28Å 126.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 1.72 24.43 – 1.72	Depositor EDS
% Data completeness (in resolution range)	85.4 (24.90-1.72) 85.5 (24.43-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.73Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.277 0.234 , 0.284	Depositor DCC
R_{free} test set	2812 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4060	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 2W5, ADP

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	0.96	0/1261	0.99	4/1700 (0.2%)
1	B	0.88	0/1287	0.95	5/1733 (0.3%)
1	C	0.89	1/1278 (0.1%)	0.98	1/1721 (0.1%)
All	All	0.91	1/3826 (0.0%)	0.97	10/5154 (0.2%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	98	GLU	CD-OE2	6.69	1.33	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	VAL	CG1-CB-CG2	6.93	121.98	110.90
1	A	136	VAL	CG1-CB-CG2	6.88	121.91	110.90
1	A	132	ILE	CB-CA-C	-5.89	99.82	111.60
1	B	29	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	B	71	PHE	C-N-CA	5.34	135.04	121.70
1	A	142	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	45	GLY	N-CA-C	-5.19	100.11	113.10
1	B	82	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	C	29	ARG	NE-CZ-NH2	5.04	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	PHE	CA-C-N	5.04	128.28	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	PHE	Peptide
1	A	2	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1235	0	1240	33	0
1	B	1261	0	1271	26	0
1	C	1252	0	1265	22	0
2	A	28	0	21	0	0
2	B	28	0	23	2	0
2	C	28	0	23	3	0
3	A	15	0	18	1	0
3	B	15	0	18	0	0
4	A	27	0	12	0	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
5	A	35	0	0	2	0
5	B	40	0	0	0	0
5	C	42	0	0	1	0
All	All	4060	0	3915	83	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 11.

All (83) 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:46:THR:HG21	1:A:134:LYS:HD3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:O	1:B:39:LYS:HD2	1.70	0.90
1:B:16:THR:H	1:B:19:HIS:HD2	1.21	0.89
4:B:203:ADP:O2'	4:B:203:ADP:N3	2.13	0.81
1:A:16:THR:H	1:A:19:HIS:HD2	1.30	0.80
1:A:46:THR:HG21	1:A:134:LYS:CD	2.16	0.74
1:B:38:LEU:HD12	1:B:38:LEU:H	1.51	0.73
1:C:46:THR:HG21	1:C:134:LYS:HD2	1.73	0.71
1:A:156:LYS:O	1:A:160:LYS:HA	1.91	0.70
1:B:136:VAL:HG13	1:B:141:ALA:HB3	1.74	0.68
1:C:46:THR:HG21	1:C:134:LYS:CD	2.25	0.66
1:A:128:ILE:HA	1:A:132:ILE:HD11	1.77	0.66
1:B:16:THR:H	1:B:19:HIS:CD2	2.10	0.64
1:B:103:LEU:HD22	2:B:201:2W5:H8	1.81	0.63
1:C:16:THR:H	1:C:19:HIS:HD2	1.47	0.62
1:C:22:ILE:CD1	1:C:90:GLY:HA3	2.29	0.61
1:A:121:SER:HB2	5:A:310:HOH:O	2.01	0.61
1:C:36[A]:CYS:SG	1:C:78:TYR:CE2	2.94	0.61
1:A:77:ASP:OD1	3:A:202:EPE:H71	2.01	0.60
1:B:16:THR:N	1:B:19:HIS:HD2	1.95	0.60
4:C:202:ADP:H5'2	4:C:202:ADP:PB	2.41	0.60
1:C:160:LYS:CD	1:C:160:LYS:O	2.51	0.59
1:B:65:ASN:H	1:B:65:ASN:HD22	1.53	0.56
1:C:32:GLU:OE1	1:C:67:LYS:NZ	2.38	0.56
1:A:7:VAL:HG13	1:A:36[A]:CYS:SG	2.45	0.56
1:A:38:LEU:N	1:A:38:LEU:CD1	2.68	0.56
1:A:37:VAL:HG12	1:A:38:LEU:N	2.20	0.56
1:C:160:LYS:O	1:C:160:LYS:HD2	2.06	0.56
1:A:2:GLU:HA	1:A:31:ASP:HB2	1.89	0.55
1:C:30:PHE:CE2	1:C:88:ILE:HD11	2.41	0.54
1:B:73:GLY:O	2:B:201:2W5:H23	2.08	0.54
1:B:46:THR:HG21	1:B:134:LYS:HD2	1.89	0.53
1:B:76:VAL:CG2	1:B:111:ASN:HB3	2.38	0.53
1:B:106:MET:CE	1:C:132:ILE:HD13	2.39	0.53
1:A:38:LEU:N	1:A:38:LEU:HD12	2.23	0.52
1:A:2:GLU:HB3	1:A:32:GLU:OE2	2.10	0.52
1:B:65:ASN:N	1:B:65:ASN:HD22	2.08	0.52
1:C:16:THR:H	1:C:19:HIS:CD2	2.27	0.51
1:C:136:VAL:HG13	1:C:141:ALA:HB3	1.94	0.50
1:C:7:VAL:HG13	1:C:36[A]:CYS:SG	2.52	0.49
1:A:16:THR:H	1:A:19:HIS:CD2	2.19	0.49
1:A:34:HIS:HD2	1:A:78:TYR:OH	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:H	1:A:38:LEU:CD1	2.27	0.48
1:C:29:ARG:HH11	1:C:29:ARG:HG3	1.77	0.48
1:A:136:VAL:HG23	2:C:201:2W5:H13	1.96	0.47
2:C:201:2W5:H1	4:C:202:ADP:O2A	2.14	0.47
1:C:145:GLU:HG2	1:C:146:PHE:CE1	2.50	0.47
1:B:76:VAL:HG22	1:B:111:ASN:HB3	1.96	0.46
1:A:10:GLY:O	1:A:38:LEU:HD13	2.15	0.46
1:A:25:ARG:HB2	1:A:119:MET:HE1	1.97	0.46
1:A:36[A]:CYS:SG	1:A:78:TYR:CE2	3.09	0.45
1:C:145:GLU:CG	1:C:146:PHE:CE1	2.99	0.45
1:A:20:LEU:HD11	1:A:148:PRO:HG3	1.98	0.45
1:B:39:LYS:N	1:B:71:PHE:O	2.50	0.45
1:B:71:PHE:HA	1:B:72:SER:HB2	1.98	0.45
1:B:38:LEU:O	1:B:39:LYS:CD	2.56	0.45
1:B:71:PHE:HA	1:B:72:SER:CB	2.47	0.45
1:C:145:GLU:HG2	1:C:146:PHE:CD1	2.52	0.44
1:A:32:GLU:OE1	1:A:34:HIS:HE1	2.00	0.44
1:A:29:ARG:HG3	1:A:29:ARG:NH1	2.33	0.44
1:B:29:ARG:HG3	1:B:29:ARG:NH1	2.31	0.44
1:A:46:THR:CG2	1:A:134:LYS:HD3	2.33	0.44
1:A:123:THR:HG23	5:A:334:HOH:O	2.16	0.44
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.82	0.44
1:A:16:THR:N	1:A:19:HIS:HD2	2.07	0.44
1:B:34:HIS:HD2	1:B:78:TYR:OH	2.00	0.44
1:C:103:LEU:HD22	2:C:201:2W5:H8	2.01	0.43
1:B:88:ILE:HD13	1:B:117:LEU:HB2	2.00	0.43
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.84	0.43
1:B:159:PHE:O	1:B:160:LYS:HB2	2.18	0.43
1:B:12:PHE:N	4:B:203:ADP:O3B	2.30	0.42
1:C:128:ILE:HA	1:C:132:ILE:HD11	2.01	0.42
1:B:76:VAL:HG21	1:B:111:ASN:HB3	2.01	0.42
1:A:92:ARG:NH2	1:A:128:ILE:O	2.52	0.42
1:C:159:PHE:O	1:C:160:LYS:C	2.58	0.41
1:A:88:ILE:HD13	1:A:117:LEU:HB2	2.03	0.41
1:A:37:VAL:CG1	1:A:38:LEU:N	2.83	0.41
1:A:46:THR:HG23	1:A:47:PHE:CD2	2.55	0.41
1:C:128:ILE:HG21	1:C:128:ILE:HD13	1.86	0.41
1:A:34:HIS:CE1	1:A:67:LYS:HE3	2.55	0.40
1:A:2:GLU:CD	1:A:32:GLU:OE2	2.60	0.40
1:C:89:ARG:HD2	5:C:332:HOH:O	2.22	0.40
1:B:46:THR:HG23	1:B:134:LYS:NZ	2.36	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	150/160 (94%)	150 (100%)	0	0	100	100
1	B	153/160 (96%)	149 (97%)	3 (2%)	1 (1%)	22	8
1	C	152/160 (95%)	149 (98%)	3 (2%)	0	100	100
All	All	455/480 (95%)	448 (98%)	6 (1%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	SER

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	141/147 (96%)	133 (94%)	8 (6%)	20	6
1	B	144/147 (98%)	127 (88%)	17 (12%)	5	1
1	C	143/147 (97%)	131 (92%)	12 (8%)	11	2
All	All	428/441 (97%)	391 (91%)	37 (9%)	10	2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	64	PRO
1	A	65	ASN
1	A	76	VAL
1	A	115	GLU
1	A	121	SER
1	A	132	ILE
1	A	136	VAL
1	B	1	MET
1	B	2	GLU
1	B	14	PRO
1	B	34	HIS
1	B	38	LEU
1	B	39	LYS
1	B	44	GLU
1	B	46	THR
1	B	65	ASN
1	B	76	VAL
1	B	80	GLU
1	B	82	VAL
1	B	108	LYS
1	B	122	SER
1	B	135	GLU
1	B	140	ARG
1	B	160	LYS
1	C	34	HIS
1	C	37	VAL
1	C	65	ASN
1	C	70	GLN
1	C	81	GLN
1	C	82	VAL
1	C	92	ARG
1	C	112	ASN
1	C	117	LEU
1	C	128	ILE
1	C	131	SER
1	C	160	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	34	HIS

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Mol	Chain	Res	Type
1	A	62	HIS
1	A	65	ASN
1	A	69	HIS
1	A	107	ASN
1	B	19	HIS
1	B	34	HIS
1	B	65	ASN
1	B	107	ASN
1	C	19	HIS
1	C	34	HIS
1	C	65	ASN
1	C	69	HIS
1	C	70	GLN
1	C	107	ASN
1	C	112	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
4	ADP	A	203	-	24,29,29	1.32	3 (12%)	29,45,45	2.49	10 (34%)
2	2W5	B	201	-	29,30,30	1.77	5 (17%)	38,41,41	4.81	20 (52%)
3	EPE	B	202	-	15,15,15	1.44	1 (6%)	18,20,20	2.64	6 (33%)
2	2W5	A	201	-	29,30,30	1.13	2 (6%)	38,41,41	3.90	19 (50%)
2	2W5	C	201	-	29,30,30	1.50	5 (17%)	38,41,41	4.49	15 (39%)
3	EPE	A	202	-	15,15,15	1.75	2 (13%)	18,20,20	2.20	6 (33%)
4	ADP	B	203	-	24,29,29	1.87	7 (29%)	29,45,45	2.41	12 (41%)
4	ADP	C	202	-	24,29,29	1.50	5 (20%)	29,45,45	1.44	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	203	-	-	5/12/32/32	0/3/3/3
2	2W5	B	201	-	-	8/15/28/28	0/3/3/3
3	EPE	B	202	-	-	2/9/19/19	0/1/1/1
2	2W5	A	201	-	2/2/3/4	3/15/28/28	0/3/3/3
2	2W5	C	201	-	-	5/15/28/28	0/3/3/3
3	EPE	A	202	-	-	4/9/19/19	0/1/1/1
4	ADP	B	203	-	-	6/12/32/32	0/3/3/3
4	ADP	C	202	-	-	7/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	EPE	C10-S	-5.87	1.69	1.77
3	B	202	EPE	C10-S	-5.16	1.70	1.77
4	B	203	ADP	O4'-C1'	4.89	1.47	1.41
2	B	201	2W5	C30-C28	4.39	1.45	1.38
2	C	201	2W5	C17-C11	-4.09	1.49	1.55
2	B	201	2W5	C30-C23	4.04	1.46	1.39
4	C	202	ADP	O4'-C1'	3.82	1.46	1.41
2	B	201	2W5	C4-C5	3.63	1.44	1.38
4	B	203	ADP	C2-N3	3.37	1.37	1.32
4	C	202	ADP	C2-N3	3.08	1.37	1.32
4	B	203	ADP	C5-C4	3.06	1.49	1.40
4	A	203	ADP	C5-C4	3.00	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	2W5	O20-C19	-2.92	1.17	1.23
2	C	201	2W5	C13-C11	2.90	1.57	1.53
2	C	201	2W5	C4-C5	2.90	1.43	1.38
2	A	201	2W5	C4-C3	2.88	1.43	1.38
4	B	203	ADP	C4-N3	2.82	1.39	1.35
4	A	203	ADP	O4'-C1'	2.75	1.44	1.41
2	A	201	2W5	C17-C11	-2.58	1.51	1.55
4	C	202	ADP	C5-C4	2.45	1.47	1.40
2	B	201	2W5	O6-C5	2.43	1.39	1.35
4	A	203	ADP	C2-N3	2.42	1.36	1.32
3	A	202	EPE	O2S-S	2.39	1.52	1.45
4	B	203	ADP	C8-N7	2.19	1.38	1.34
2	B	201	2W5	C4-C3	2.06	1.41	1.38
4	C	202	ADP	PB-O1B	2.05	1.57	1.50
2	C	201	2W5	O2-C3	-2.05	1.31	1.35
4	B	203	ADP	C2'-C1'	2.05	1.56	1.53
4	B	203	ADP	C6-C5	2.05	1.50	1.43
4	C	202	ADP	C4-N3	2.02	1.38	1.35

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	2W5	O20-C19-C17	-14.62	104.12	121.73
2	B	201	2W5	C11-C9-N8	13.38	130.71	117.00
2	C	201	2W5	C11-C9-N8	11.98	129.27	117.00
2	A	201	2W5	C16-C17-C11	11.23	122.08	109.58
2	C	201	2W5	C17-C19-N21	11.09	134.17	116.24
2	B	201	2W5	C30-C28-CL9	10.86	136.03	118.49
2	B	201	2W5	C22-C23-C24	-10.60	98.91	120.91
2	A	201	2W5	C11-C9-N10	8.62	125.83	117.00
2	B	201	2W5	C22-C23-C30	8.40	138.80	120.64
4	A	203	ADP	O5'-C5'-C4'	-7.96	81.58	108.99
2	B	201	2W5	C28-C30-C23	-7.80	115.14	120.46
3	B	202	EPE	O1S-S-C10	7.77	116.27	106.92
2	C	201	2W5	C11-C9-N10	-7.65	109.17	117.00
2	B	201	2W5	O20-C19-C17	-7.62	112.55	121.73
2	A	201	2W5	C11-C9-N8	-7.47	109.34	117.00
2	A	201	2W5	O20-C19-C17	-7.42	112.78	121.73
2	B	201	2W5	C11-C9-N10	-7.16	109.67	117.00
2	A	201	2W5	C11-C17-C19	6.87	120.78	111.21
2	C	201	2W5	C16-C17-C11	6.29	116.58	109.58
2	B	201	2W5	C26-C28-CL9	-6.24	105.61	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	2W5	C4-C5-N8	-6.11	116.94	124.08
3	A	202	EPE	O2S-S-C10	6.07	114.22	106.92
2	C	201	2W5	C1-O2-C3	-5.92	108.08	117.36
2	A	201	2W5	C7-O6-C5	-5.65	108.50	117.36
2	A	201	2W5	C22-N21-C19	-5.57	114.33	122.34
4	B	203	ADP	N3-C2-N1	-5.55	120.01	128.68
4	B	203	ADP	C3'-C2'-C1'	5.46	109.20	100.98
4	A	203	ADP	C2'-C3'-C4'	-5.36	92.22	102.64
2	C	201	2W5	C11-C17-C19	5.11	118.33	111.21
4	B	203	ADP	C1'-N9-C4	-5.02	117.83	126.64
2	B	201	2W5	N10-C9-N8	-4.99	118.80	126.00
3	B	202	EPE	O2S-S-C10	-4.97	100.93	106.92
4	B	203	ADP	O4'-C1'-C2'	-4.78	99.95	106.93
2	B	201	2W5	C4-C5-N8	-4.70	118.60	124.08
2	B	201	2W5	C4-C3-N10	-4.68	118.62	124.08
2	B	201	2W5	C22-N21-C19	4.64	129.01	122.34
2	A	201	2W5	C5-C4-C3	4.36	119.17	115.21
2	C	201	2W5	C7-O6-C5	-4.32	110.58	117.36
2	C	201	2W5	C4-C5-N8	-4.30	119.06	124.08
2	B	201	2W5	C16-C17-C11	4.25	114.31	109.58
2	A	201	2W5	C17-C19-N21	4.15	122.95	116.24
4	C	202	ADP	N3-C2-N1	-4.11	122.26	128.68
2	C	201	2W5	C22-N21-C19	-3.87	116.78	122.34
2	B	201	2W5	C23-C22-N21	3.86	121.32	113.05
4	A	203	ADP	N3-C2-N1	-3.84	122.68	128.68
4	A	203	ADP	PA-O3A-PB	-3.77	119.88	132.83
2	C	201	2W5	N10-C9-N8	-3.70	120.66	126.00
2	C	201	2W5	C28-C30-C23	-3.61	117.99	120.46
4	A	203	ADP	C3'-C2'-C1'	3.59	106.39	100.98
2	B	201	2W5	C1-O2-C3	-3.58	111.75	117.36
2	C	201	2W5	C4-C3-N10	-3.37	120.14	124.08
2	A	201	2W5	C14-C13-C11	-3.26	107.15	111.63
4	B	203	ADP	O2B-PB-O3A	3.15	115.19	104.64
3	A	202	EPE	O1S-S-C10	-3.12	103.16	106.92
2	A	201	2W5	C13-C11-C17	3.09	114.85	109.84
3	A	202	EPE	O3S-S-O2S	-3.02	103.89	111.27
3	B	202	EPE	C3-C2-N1	2.93	116.66	110.64
2	B	201	2W5	O20-C19-N21	2.92	129.26	122.99
4	A	203	ADP	O4'-C4'-C3'	2.91	110.87	105.11
2	A	201	2W5	C24-C23-C30	2.86	122.55	118.54
4	B	203	ADP	C2'-C3'-C4'	-2.83	97.15	102.64
4	C	202	ADP	PA-O3A-PB	2.82	142.51	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	EPE	O2S-S-O1S	-2.78	104.31	113.95
3	B	202	EPE	C9-N1-C2	-2.69	104.35	111.23
4	A	203	ADP	N6-C6-N1	2.63	124.03	118.57
4	B	203	ADP	C4-C5-N7	-2.63	106.66	109.40
2	A	201	2W5	C4-C3-N10	-2.60	121.04	124.08
2	B	201	2W5	C25-C26-CL7	-2.60	113.19	118.41
2	A	201	2W5	C16-C17-C19	2.60	117.12	111.13
2	B	201	2W5	C24-C23-C30	2.58	122.15	118.54
4	A	203	ADP	C5'-C4'-C3'	2.55	124.73	115.18
2	A	201	2W5	C15-C14-C13	-2.54	106.23	111.42
4	B	203	ADP	C2-N1-C6	2.51	123.06	118.75
3	A	202	EPE	C6-C5-N4	2.46	115.69	110.64
3	A	202	EPE	C2-C3-N4	2.43	115.62	110.64
2	C	201	2W5	C24-C23-C30	2.40	121.90	118.54
2	A	201	2W5	C22-C23-C30	-2.39	115.48	120.64
4	A	203	ADP	C2-N1-C6	2.32	122.73	118.75
4	B	203	ADP	O3A-PB-O1B	-2.32	98.35	111.19
4	B	203	ADP	O5'-C5'-C4'	-2.31	101.03	108.99
3	B	202	EPE	O3S-S-O1S	2.30	116.89	111.27
4	A	203	ADP	O2A-PA-O1A	2.28	123.53	112.24
2	B	201	2W5	C5-C4-C3	2.27	117.27	115.21
2	B	201	2W5	O6-C5-N8	2.15	123.55	118.12
2	A	201	2W5	C15-C16-C17	2.13	115.47	111.77
4	B	203	ADP	O4'-C4'-C5'	2.07	116.19	109.37
4	B	203	ADP	O3'-C3'-C4'	2.06	117.00	111.05
3	A	202	EPE	C5-N4-C3	2.04	113.42	108.83
2	A	201	2W5	C25-C24-C23	-2.02	118.24	121.03
2	C	201	2W5	O2-C3-C4	2.00	124.38	118.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	201	2W5	C17
2	A	201	2W5	C11

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	ADP	PB-O3A-PA-O5'
4	A	203	ADP	C5'-O5'-PA-O3A
4	A	203	ADP	C3'-C4'-C5'-O5'
2	B	201	2W5	C13-C11-C9-N10

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Mol	Chain	Res	Type	Atoms
3	B	202	EPE	S-C10-C9-N1
2	C	201	2W5	C13-C11-C9-N10
3	A	202	EPE	C10-C9-N1-C2
4	B	203	ADP	C5'-O5'-PA-O2A
4	C	202	ADP	C5'-O5'-PA-O2A
4	C	202	ADP	C5'-O5'-PA-O3A
2	B	201	2W5	C23-C22-N21-C19
2	A	201	2W5	C4-C5-O6-C7
2	B	201	2W5	N8-C5-O6-C7
2	A	201	2W5	N8-C5-O6-C7
4	B	203	ADP	C3'-C4'-C5'-O5'
2	B	201	2W5	C4-C5-O6-C7
4	A	203	ADP	O4'-C4'-C5'-O5'
4	B	203	ADP	C4'-C5'-O5'-PA
4	B	203	ADP	PB-O3A-PA-O5'
4	C	202	ADP	PB-O3A-PA-O5'
4	C	202	ADP	O4'-C4'-C5'-O5'
4	A	203	ADP	C5'-O5'-PA-O1A
4	C	202	ADP	C5'-O5'-PA-O1A
3	A	202	EPE	C9-C10-S-O3S
3	A	202	EPE	C9-C10-S-O1S
2	B	201	2W5	C11-C17-C19-O20
4	C	202	ADP	C4'-C5'-O5'-PA
2	C	201	2W5	C16-C17-C19-O20
3	B	202	EPE	C10-C9-N1-C6
2	C	201	2W5	N8-C5-O6-C7
2	B	201	2W5	C16-C17-C19-O20
2	A	201	2W5	C11-C17-C19-O20
2	C	201	2W5	C11-C17-C19-O20
2	B	201	2W5	C11-C17-C19-N21
2	C	201	2W5	C11-C17-C19-N21
4	B	203	ADP	C5'-O5'-PA-O3A
4	B	203	ADP	C5'-O5'-PA-O1A
3	A	202	EPE	C9-C10-S-O2S
2	B	201	2W5	C16-C17-C19-N21
4	C	202	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 9 short contacts:

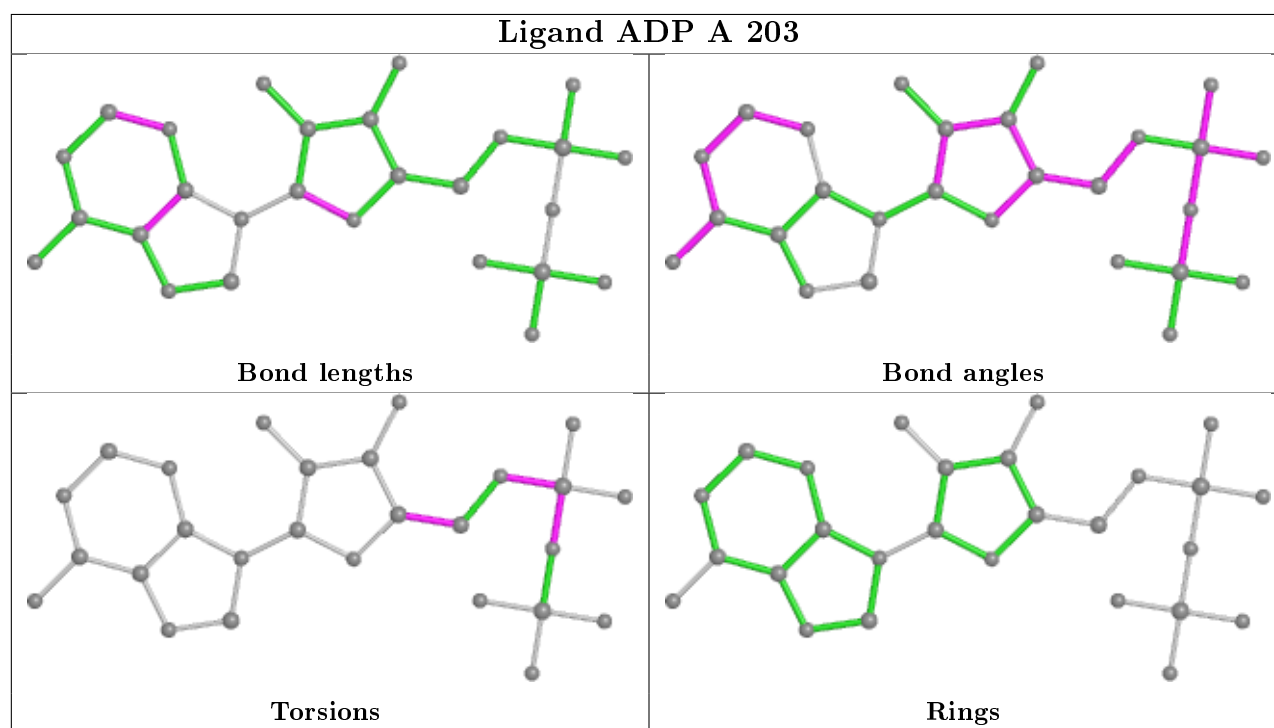
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	2W5	2	0

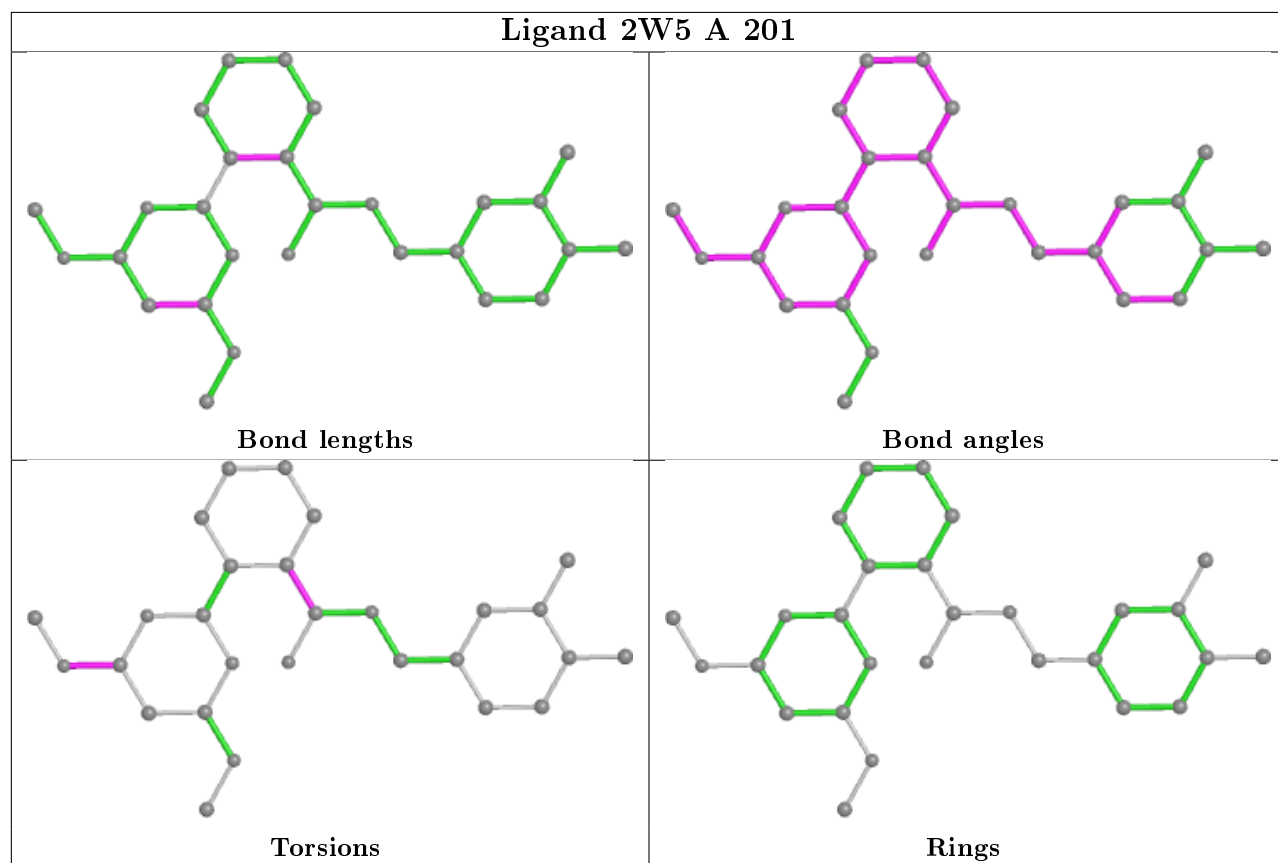
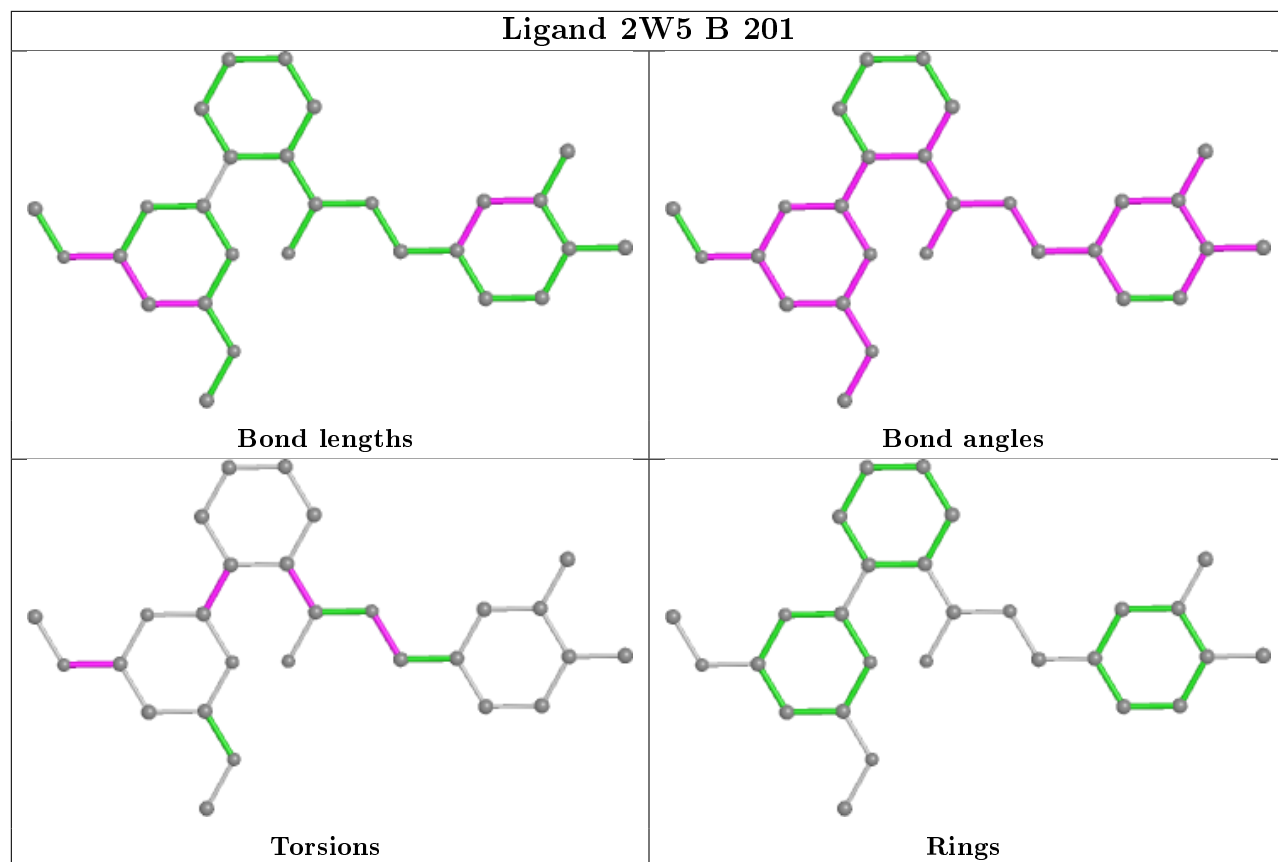
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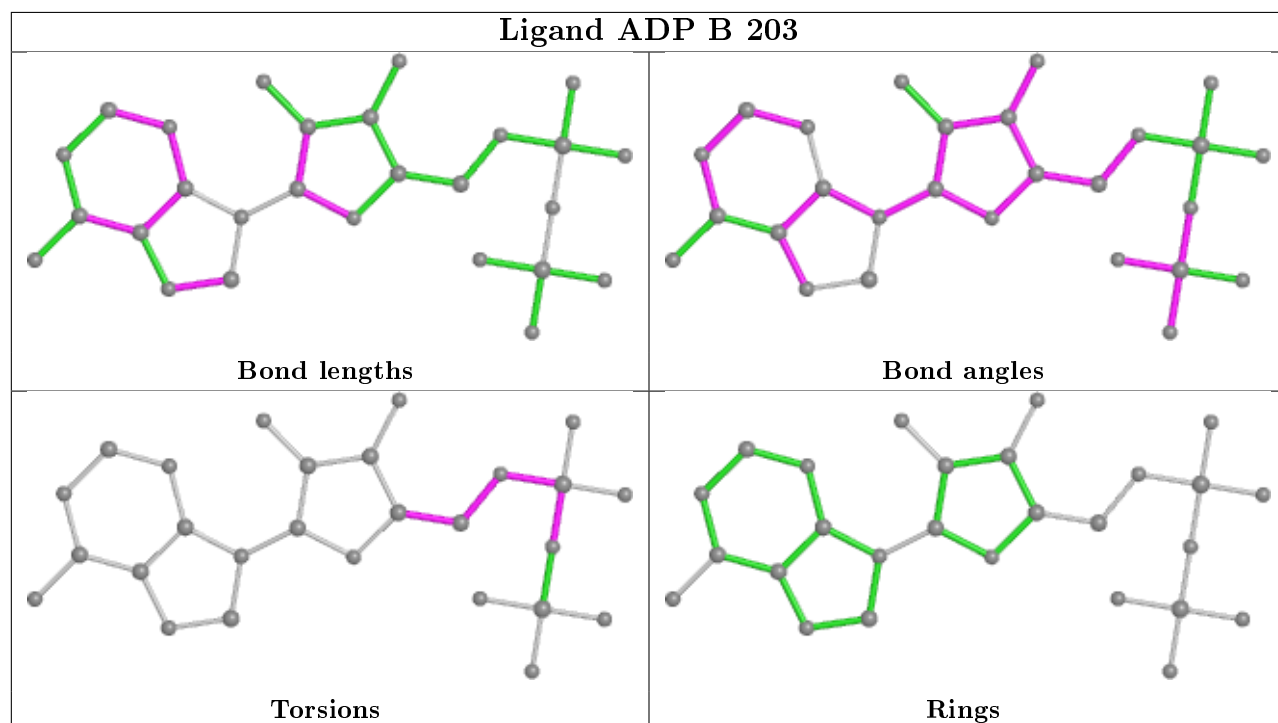
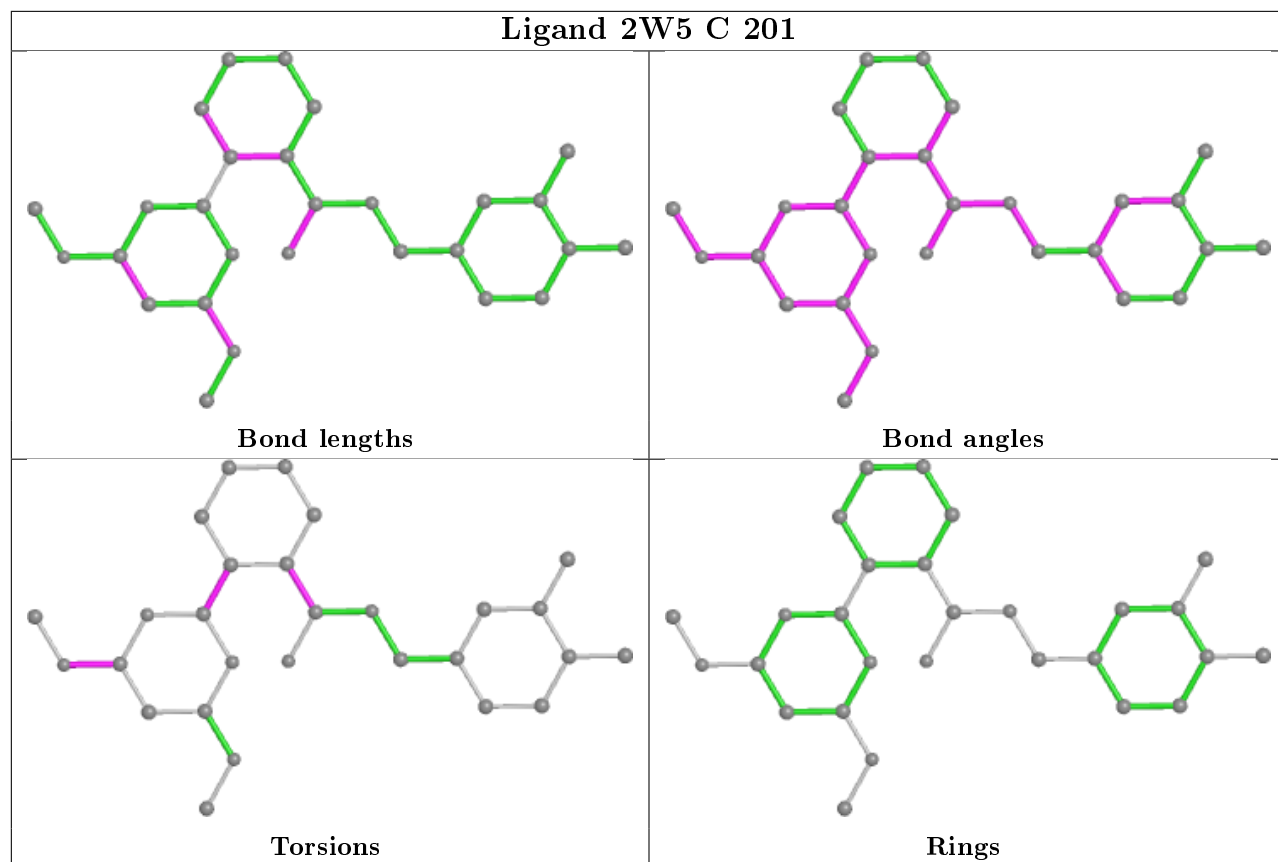
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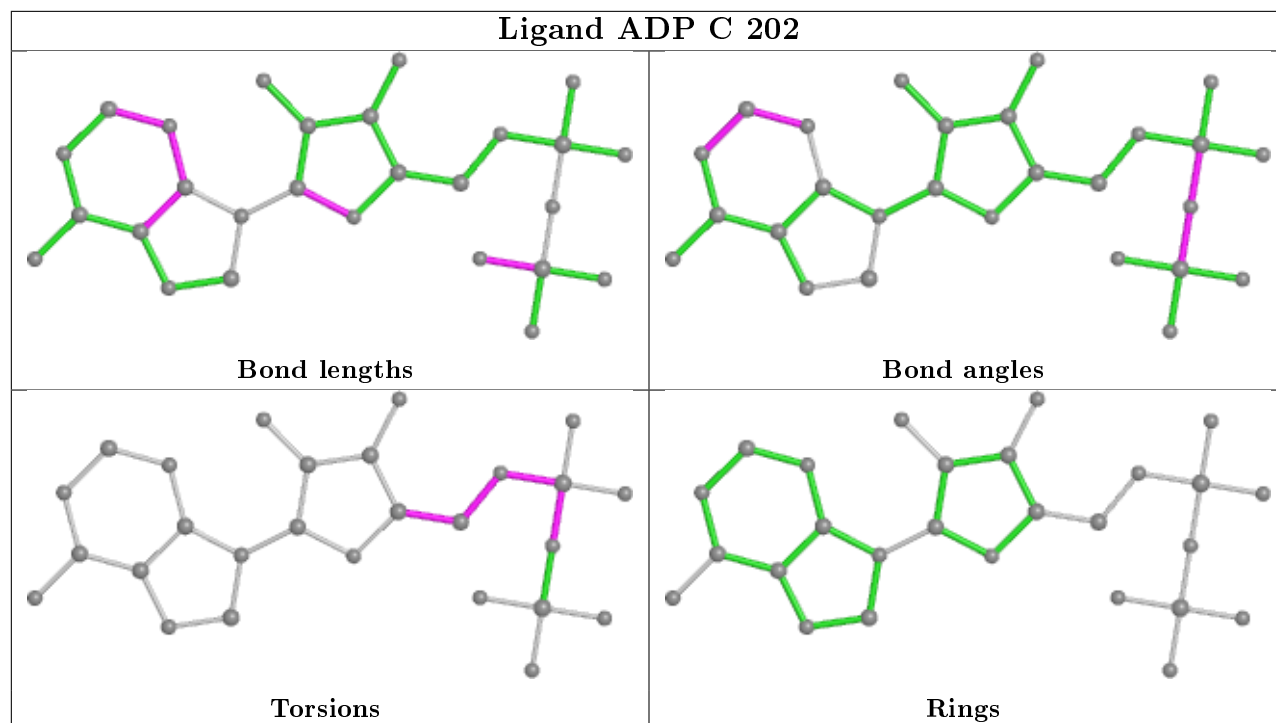
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	2W5	3	0
3	A	202	EPE	1	0
4	B	203	ADP	2	0
4	C	202	ADP	2	0

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









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	153/160 (95%)	0.46	9 (5%) 22 24	22, 30, 43, 50	0
1	B	156/160 (97%)	0.47	13 (8%) 11 13	23, 33, 49, 50	0
1	C	155/160 (96%)	0.53	17 (10%) 5 6	24, 34, 46, 50	0
All	All	464/480 (96%)	0.48	39 (8%) 11 12	22, 32, 46, 50	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	GLU	5.3
1	B	1	MET	5.1
1	A	38	LEU	4.5
1	A	72	SER	4.4
1	C	8	ILE	3.7
1	A	45	GLY	3.7
1	B	2	GLU	3.6
1	C	88	ILE	3.3
1	C	160	LYS	3.3
1	C	22	ILE	3.2
1	B	15	ILE	3.1
1	B	38	LEU	3.1
1	B	8	ILE	3.0
1	B	45	GLY	2.8
1	C	15	ILE	2.6
1	C	1	MET	2.6
1	B	39	LYS	2.6
1	A	35	VAL	2.6
1	B	35	VAL	2.6
1	A	8	ILE	2.5
1	C	142	ASP	2.5
1	A	15	ILE	2.5
1	A	36[A]	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	112	ASN	2.4
1	C	118	TYR	2.4
1	A	87	ILE	2.3
1	C	23	ILE	2.3
1	C	117	LEU	2.3
1	A	2	GLU	2.3
1	C	61	LYS	2.3
1	B	160	LYS	2.2
1	B	88	ILE	2.1
1	C	35	VAL	2.1
1	B	117	LEU	2.1
1	C	12	PHE	2.1
1	C	45	GLY	2.1
1	C	123	THR	2.1
1	C	92	ARG	2.0
1	C	50	GLU	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.

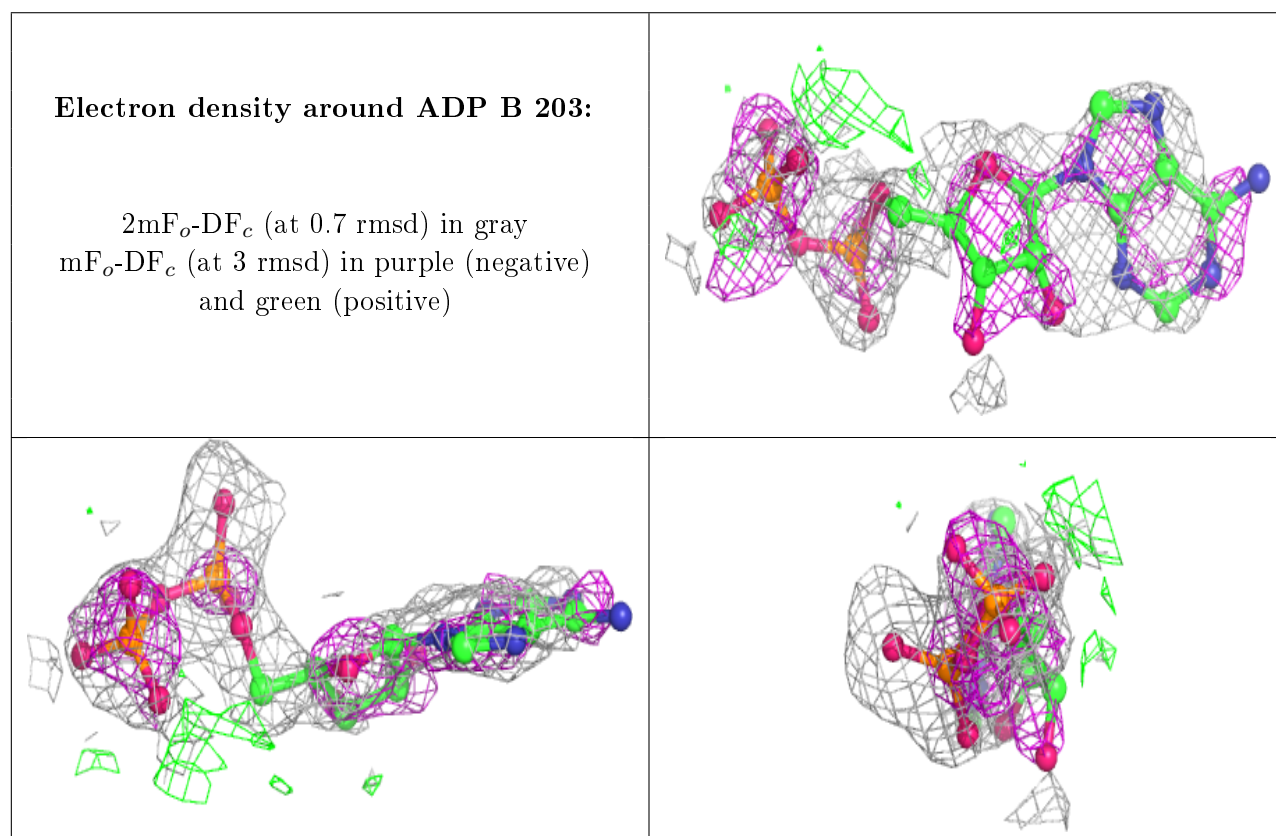
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ADP	B	203	27/27	0.73	0.45	45,50,50,50	0
4	ADP	A	203	27/27	0.81	0.39	49,50,50,50	0
3	EPE	A	202	15/15	0.82	0.17	43,46,50,50	0
2	2W5	B	201	28/28	0.83	0.14	29,36,50,50	0
4	ADP	C	202	27/27	0.83	0.38	46,50,50,50	0
2	2W5	C	201	28/28	0.90	0.10	25,32,45,50	0
2	2W5	A	201	28/28	0.90	0.09	28,34,44,50	0

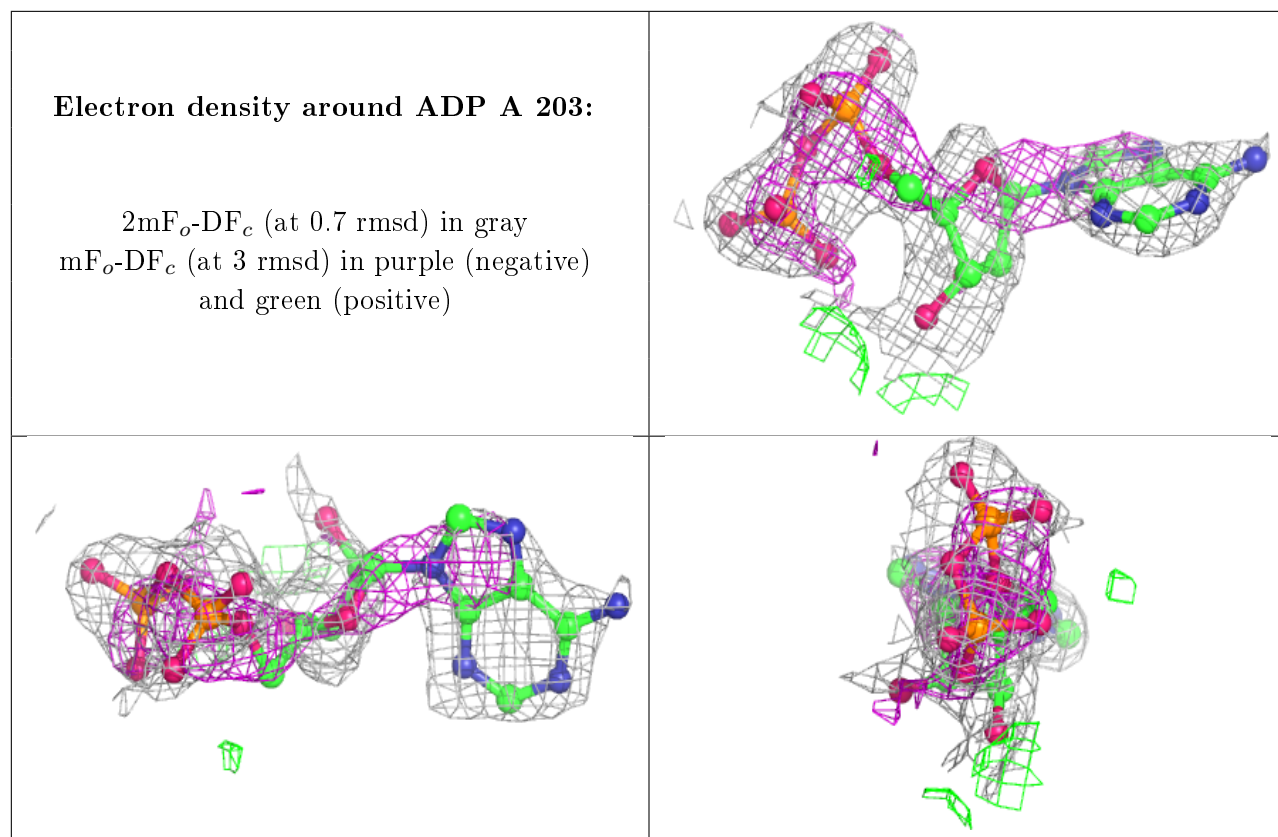
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EPE	B	202	15/15	0.93	0.09	28,33,50,50	0

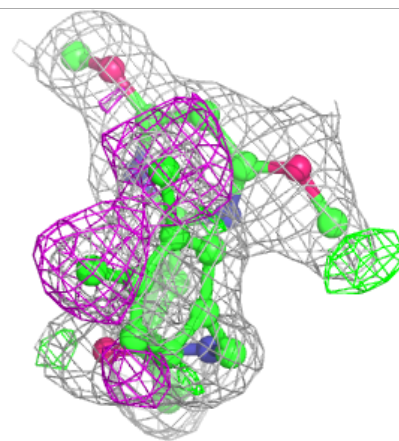
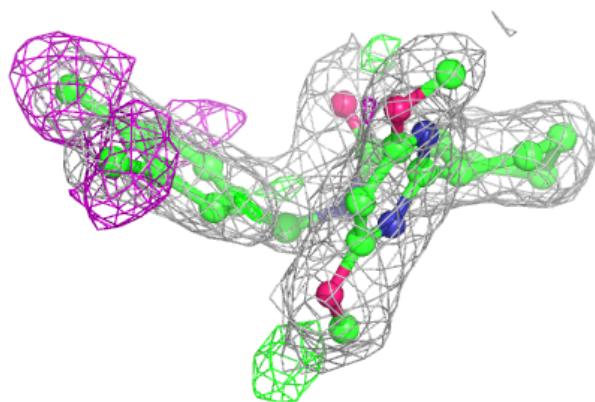
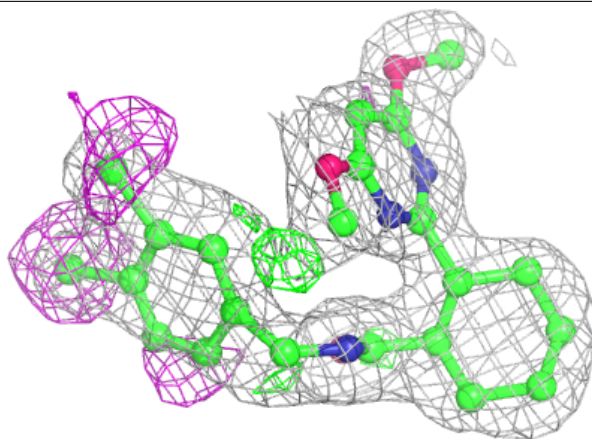
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

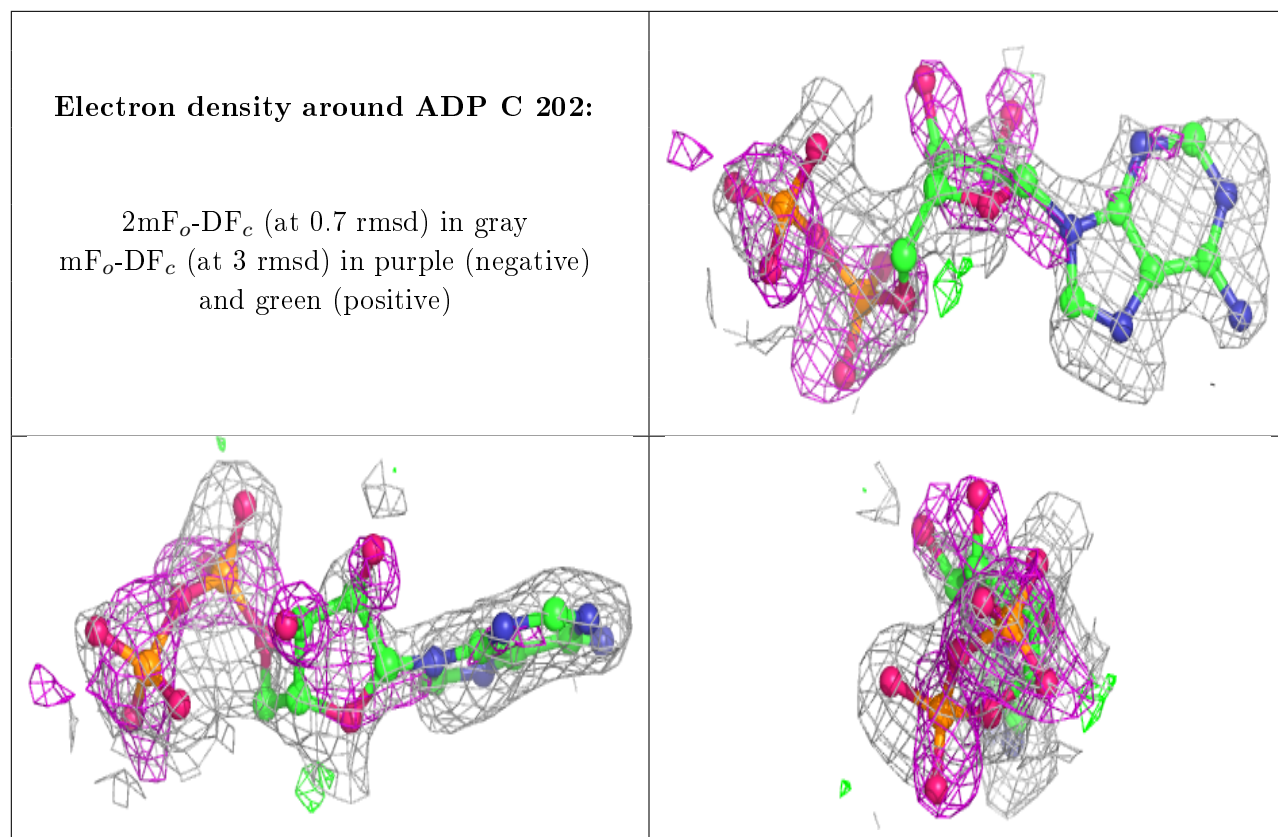




Electron density around 2W5 B 201:

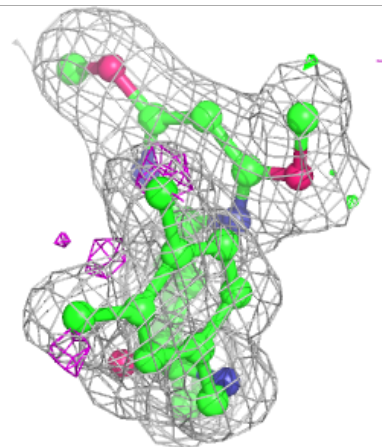
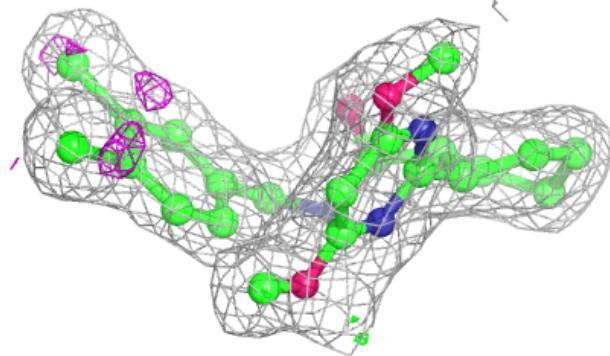
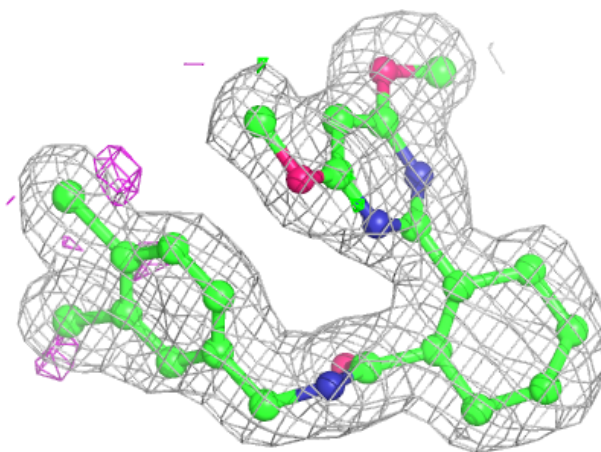
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

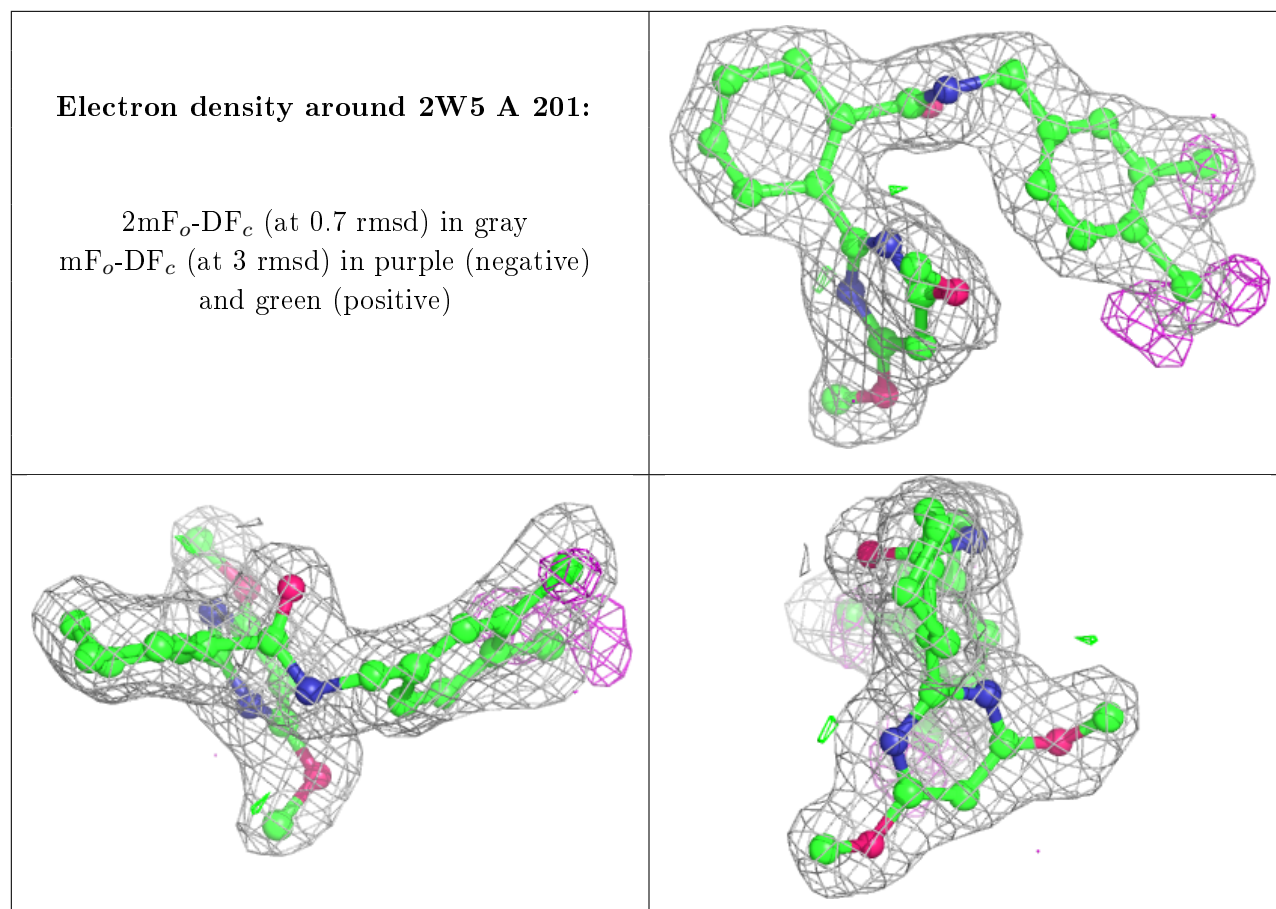




Electron density around 2W5 C 201:

$2mF_o-DF_c$ (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.