Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 12:43 pm BST

PDB ID	:	3CWQ
Title	:	Crystal structure of chromosome partitioning protein (ParA) in complex with ADP from Synechocystis sp. Northeast Structural Genomics Consortium Target SgR89
Authors	:	Forouhar, F.; Neely, H.; Seetharaman, J.; Mao, L.; Xiao, R.; Janjua, H.; Maglaqui, M.; Foote, E.L.; Lee, D.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-04-22
Resolution	:	2.47 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

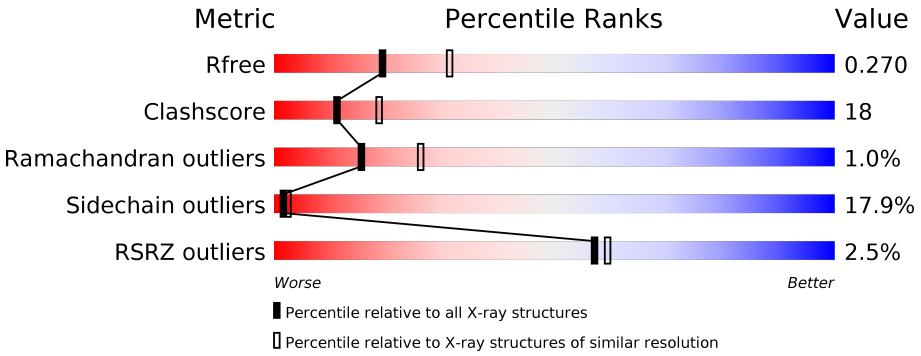
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	209	3% 54% 33% 10% ••
1	B	209	% 55% 28% 11% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3167 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.

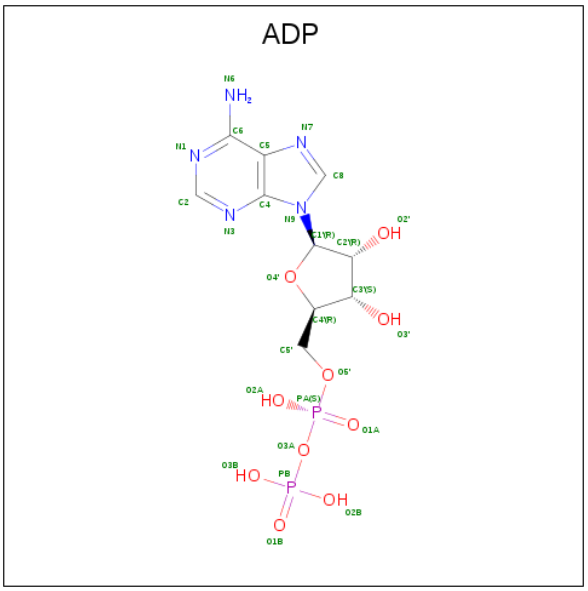
- Molecule 1 is a protein called ParA family chromosome partitioning protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	Se	0	0	0
			1577	1002	269	303	1	2			
1	B	197	Total	C	N	O	S	Se	0	0	0
			1497	954	254	286	1	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	LEU	-	EXPRESSION TAG	UNP Q6YRW8
A	203	GLU	-	EXPRESSION TAG	UNP Q6YRW8
A	204	HIS	-	EXPRESSION TAG	UNP Q6YRW8
A	205	HIS	-	EXPRESSION TAG	UNP Q6YRW8
A	206	HIS	-	EXPRESSION TAG	UNP Q6YRW8
A	207	HIS	-	EXPRESSION TAG	UNP Q6YRW8
A	208	HIS	-	EXPRESSION TAG	UNP Q6YRW8
A	209	HIS	-	EXPRESSION TAG	UNP Q6YRW8
B	202	LEU	-	EXPRESSION TAG	UNP Q6YRW8
B	203	GLU	-	EXPRESSION TAG	UNP Q6YRW8
B	204	HIS	-	EXPRESSION TAG	UNP Q6YRW8
B	205	HIS	-	EXPRESSION TAG	UNP Q6YRW8
B	206	HIS	-	EXPRESSION TAG	UNP Q6YRW8
B	207	HIS	-	EXPRESSION TAG	UNP Q6YRW8
B	208	HIS	-	EXPRESSION TAG	UNP Q6YRW8
B	209	HIS	-	EXPRESSION TAG	UNP Q6YRW8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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		

- Molecule 3 is water.

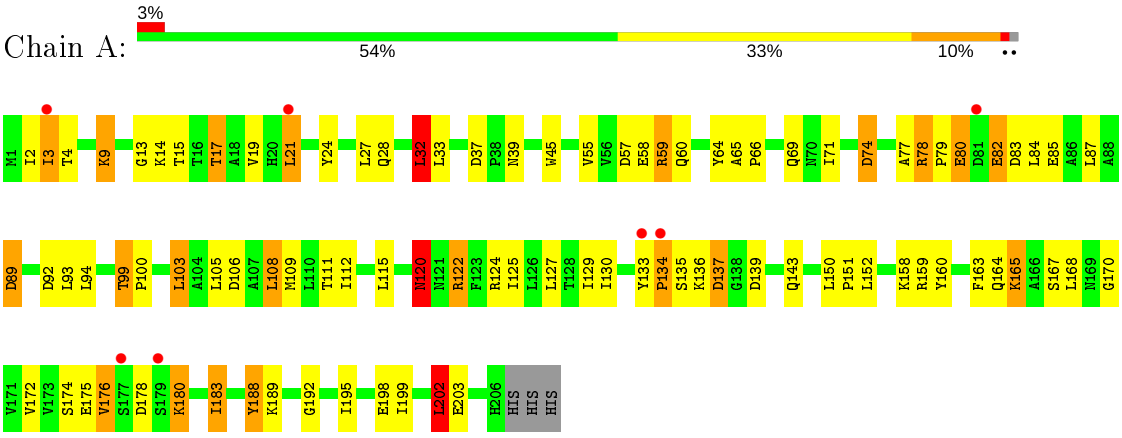
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	18	Total	O	0	0
			18	18		

3 Residue-property plots (i)

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

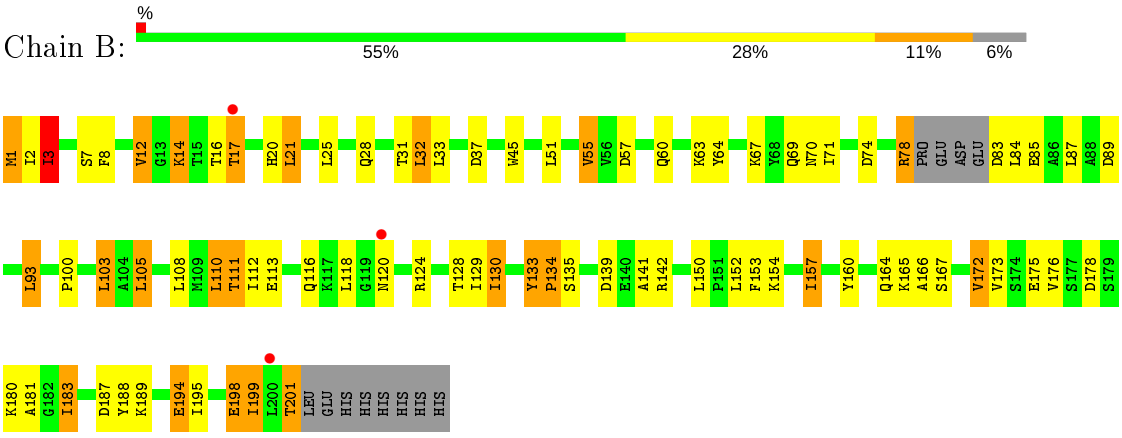
- Molecule 1: ParA family chromosome partitioning protein

Chain A:



- Molecule 1: ParA family chromosome partitioning protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.61Å 70.14Å 112.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.47 29.30 – 2.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.62-2.47) 89.7 (29.30-2.47)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	10.94 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.221 , 0.282 0.216 , 0.270	Depositor DCC
R_{free} test set	842 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3167	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.28	4/1604 (0.2%)	1.36	14/2175 (0.6%)
1	B	1.32	5/1519 (0.3%)	1.33	11/2057 (0.5%)
All	All	1.30	9/3123 (0.3%)	1.35	25/4232 (0.6%)

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	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	TYR	CE1-CZ	8.01	1.49	1.38
1	A	19	VAL	CB-CG1	7.04	1.67	1.52
1	B	194	GLU	CD-OE2	6.70	1.33	1.25
1	B	67	LYS	CD-CE	6.61	1.67	1.51
1	B	89	ASP	CB-CG	5.88	1.64	1.51
1	B	1	MSE	SE-CE	5.83	2.29	1.95
1	B	51	LEU	CG-CD1	5.30	1.71	1.51
1	A	189	LYS	CD-CE	5.23	1.64	1.51
1	A	120	ASN	CB-CG	5.07	1.62	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ASP	CB-CG-OD2	10.44	127.70	118.30
1	B	187	ASP	CB-CG-OD2	9.45	126.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	LEU	CB-CG-CD2	8.99	126.29	111.00
1	A	89	ASP	CB-CG-OD2	8.80	126.22	118.30
1	A	37	ASP	CB-CG-OD2	7.97	125.47	118.30
1	B	89	ASP	CB-CG-OD2	7.45	125.01	118.30
1	A	178	ASP	CB-CG-OD2	7.22	124.80	118.30
1	A	59	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	110	LEU	CA-CB-CG	6.82	131.00	115.30
1	B	74	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	137	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	157	ILE	CG1-CB-CG2	-6.03	98.14	111.40
1	A	32	LEU	CA-CB-CG	5.76	128.54	115.30
1	A	122	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	94	LEU	CA-CB-CG	5.67	128.33	115.30
1	B	178	ASP	CB-CG-OD2	5.64	123.37	118.30
1	A	125	ILE	CG1-CB-CG2	-5.40	99.52	111.40
1	A	103	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	B	3	ILE	CG1-CB-CG2	-5.33	99.68	111.40
1	A	106	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	139	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	32	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	83	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	105	LEU	CA-CB-CG	5.14	127.12	115.30
1	B	78	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	12	VAL	Mainchain

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	1577	0	1610	62	0
1	B	1497	0	1548	53	0
2	A	27	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	1	0
3	A	21	0	0	4	0
3	B	18	0	0	1	0
All	All	3167	0	3182	113	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 18.

All (113) 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:109:MSE:SE	1:A:109:MSE:CE	2.23	1.35
1:B:1:MSE:SE	1:B:1:MSE:CE	2.29	1.30
1:A:69:GLN:HB3	3:A:317:HOH:O	1.48	1.09
1:A:82:GLU:OE2	1:A:82:GLU:HA	1.51	1.01
1:A:124:ARG:HH11	1:A:198:GLU:HG3	1.27	0.99
1:B:133:TYR:O	1:B:135:SER:N	2.03	0.89
1:B:194:GLU:O	1:B:198:GLU:HB2	1.72	0.88
1:B:108:LEU:O	1:B:111:THR:HG22	1.80	0.81
1:B:8:PHE:CD2	1:B:108:LEU:HD12	2.18	0.79
1:A:127:LEU:HB3	1:A:130:ILE:HD11	1.66	0.77
1:A:124:ARG:NH1	1:A:198:GLU:HG3	1.98	0.77
1:A:165:LYS:HB2	1:A:176:VAL:HG21	1.68	0.75
1:A:180:LYS:HB2	1:A:183:ILE:HG22	1.71	0.73
1:B:133:TYR:O	1:B:134:PRO:C	2.28	0.70
1:B:116:GLN:O	1:B:118:LEU:N	2.24	0.68
1:B:93:LEU:HD12	1:B:195:ILE:HG23	1.75	0.68
1:B:160:TYR:OH	1:B:183:ILE:HD12	1.94	0.68
1:B:133:TYR:C	1:B:135:SER:H	1.99	0.66
1:B:103:LEU:HD23	1:B:103:LEU:H	1.60	0.66
1:B:100:PRO:HD3	1:B:128:THR:O	1.95	0.65
1:B:124:ARG:HG2	1:B:153:PHE:CE2	2.33	0.64
1:A:165:LYS:HB2	1:A:176:VAL:CG2	2.27	0.64
1:B:7:SER:HB2	1:B:12:VAL:HG21	1.79	0.63
1:A:45:TRP:CD1	1:A:170:GLY:HA2	2.34	0.63
1:B:124:ARG:NH1	1:B:198:GLU:OE2	2.31	0.62
1:A:82:GLU:OE1	1:A:85:GLU:N	2.33	0.62
1:A:202:LEU:HD22	1:A:202:LEU:O	2.00	0.61
1:A:24:TYR:O	1:A:27:LEU:HB2	2.00	0.61
1:A:99:THR:CG2	1:A:129:ILE:HD12	2.33	0.59
1:B:8:PHE:CD2	1:B:108:LEU:CD1	2.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HA	1:B:87:LEU:HD12	1.85	0.57
1:A:105:LEU:O	1:A:109:MSE:HG3	2.05	0.56
1:A:17:THR:HB	1:A:188:TYR:CE1	2.40	0.56
1:A:17:THR:HB	1:A:188:TYR:HE1	1.71	0.56
1:A:65:ALA:N	1:A:66:PRO:CD	2.69	0.56
1:A:13:GLY:O	1:A:17:THR:CG2	2.54	0.55
1:A:82:GLU:OE2	1:A:82:GLU:CA	2.41	0.55
1:A:39:ASN:OD1	3:A:308:HOH:O	2.18	0.55
1:B:173:VAL:O	1:B:176:VAL:HG12	2.06	0.55
1:A:2:ILE:HG12	1:A:71:ILE:HB	1.89	0.55
1:A:158:LYS:HB2	1:A:160:TYR:CE1	2.42	0.55
1:A:195:ILE:O	1:A:199:ILE:HG12	2.07	0.54
1:B:133:TYR:C	1:B:135:SER:N	2.59	0.54
1:B:37:ASP:HB3	3:B:303:HOH:O	2.08	0.54
1:B:183:ILE:HD13	1:B:183:ILE:O	2.09	0.53
1:A:77:ALA:O	1:A:78:ARG:HG2	2.09	0.53
1:B:124:ARG:HG2	1:B:153:PHE:CZ	2.44	0.53
1:A:112:ILE:HG12	1:A:150:LEU:HD11	1.91	0.52
1:B:8:PHE:CE2	1:B:108:LEU:HD12	2.45	0.52
1:A:13:GLY:O	1:A:17:THR:HG23	2.10	0.52
1:A:3:ILE:HG12	1:A:3:ILE:O	2.10	0.51
1:A:14:LYS:NZ	1:A:74:ASP:OD2	2.37	0.51
1:A:100:PRO:HB2	1:A:137:ASP:HB3	1.92	0.51
1:A:4:THR:HG21	1:A:87:LEU:HD22	1.92	0.51
1:A:124:ARG:HH21	1:A:151:PRO:HB2	1.75	0.51
1:A:133:TYR:O	1:A:134:PRO:C	2.49	0.51
1:B:63:LYS:HD3	1:B:64:TYR:CE1	2.45	0.50
1:B:8:PHE:HD2	1:B:108:LEU:CD1	2.22	0.50
1:B:141:ALA:O	1:B:142:ARG:C	2.49	0.50
1:B:3:ILE:HD11	1:B:25:LEU:HD11	1.93	0.50
1:A:15:THR:N	2:A:301:ADP:O1B	2.41	0.49
1:B:20:HIS:CD2	1:B:172:VAL:HG23	2.47	0.49
1:B:153:PHE:O	1:B:154:LYS:C	2.50	0.49
1:A:89:ASP:HB3	1:B:60:GLN:HE21	1.76	0.49
1:A:108:LEU:O	1:A:111:THR:HG22	2.13	0.49
1:A:120:ASN:OD1	1:A:120:ASN:N	2.46	0.48
1:B:1:MSE:N	1:B:69:GLN:O	2.46	0.48
1:B:2:ILE:HG12	1:B:71:ILE:HB	1.94	0.48
1:B:31:THR:HA	1:B:70:ASN:O	2.13	0.48
1:A:180:LYS:HB2	1:A:183:ILE:CG2	2.40	0.48
1:A:79:PRO:O	1:A:80:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLN:C	1:B:166:ALA:N	2.66	0.47
1:B:17:THR:HG22	1:B:188:TYR:OH	2.14	0.47
1:A:2:ILE:HA	1:A:71:ILE:O	2.15	0.46
1:A:9:LYS:HE3	1:A:9:LYS:HB3	1.64	0.46
1:A:139:ASP:O	1:A:143:GLN:HG3	2.16	0.46
1:B:198:GLU:O	1:B:201:THR:HG22	2.16	0.46
1:A:92:ASP:HB3	1:A:199:ILE:HD12	1.99	0.45
1:A:69:GLN:CB	3:A:317:HOH:O	2.29	0.45
1:A:13:GLY:O	1:A:17:THR:HG22	2.16	0.45
1:B:180:LYS:O	1:B:181:ALA:C	2.53	0.45
1:A:202:LEU:CD2	1:A:202:LEU:O	2.64	0.45
1:B:150:LEU:O	1:B:152:LEU:CD1	2.65	0.44
1:B:17:THR:HB	1:B:188:TYR:CE1	2.52	0.44
1:B:16:THR:HG23	1:B:45:TRP:HH2	1.82	0.44
1:B:198:GLU:O	1:B:198:GLU:OE1	2.36	0.44
1:A:60:GLN:HB3	1:A:64:TYR:CD1	2.53	0.44
1:B:7:SER:CB	1:B:12:VAL:HG21	2.45	0.43
1:B:33:LEU:O	1:B:55:VAL:HA	2.18	0.43
1:A:133:TYR:N	1:A:134:PRO:HD2	2.33	0.43
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.84	0.43
1:B:17:THR:HB	1:B:188:TYR:HE1	1.83	0.43
1:A:13:GLY:HA2	2:A:301:ADP:O1A	2.19	0.43
1:A:14:LYS:HB3	2:A:301:ADP:O1B	2.19	0.43
1:B:57:ASP:HB3	1:B:60:GLN:HG3	2.01	0.43
1:A:32:LEU:O	1:A:71:ILE:HA	2.18	0.42
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.79	0.42
1:A:180:LYS:NZ	1:A:180:LYS:HB3	2.30	0.42
1:B:133:TYR:N	1:B:134:PRO:HD2	2.35	0.42
1:A:24:TYR:CD2	1:A:192:GLY:HA3	2.54	0.42
1:B:165:LYS:HB2	1:B:176:VAL:HG21	2.02	0.41
1:A:57:ASP:HB2	3:A:318:HOH:O	2.20	0.41
1:A:14:LYS:O	1:A:15:THR:C	2.58	0.41
1:A:163:PHE:CD2	2:A:301:ADP:N6	2.88	0.41
1:A:203:GLU:OE1	1:A:203:GLU:N	2.54	0.41
1:A:65:ALA:N	1:A:66:PRO:HD2	2.35	0.41
1:B:8:PHE:CZ	1:B:111:THR:HG21	2.55	0.41
1:A:159:ARG:HA	2:A:301:ADP:N1	2.36	0.40
1:B:130:ILE:HG12	1:B:157:ILE:O	2.21	0.40
1:B:14:LYS:N	2:B:301:ADP:O1B	2.54	0.40
1:A:59:ARG:NH2	1:B:78:ARG:HG3	2.36	0.40
1:B:17:THR:O	1:B:21:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:O	1:B:199:ILE:HB	2.22	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	204/209 (98%)	185 (91%)	17 (8%)	2 (1%)	15	26
1	B	193/209 (92%)	174 (90%)	17 (9%)	2 (1%)	15	26
All	All	397/418 (95%)	359 (90%)	34 (9%)	4 (1%)	15	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	PRO
1	B	134	PRO
1	A	78	ARG
1	B	112	ILE

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	169/170 (99%)	137 (81%)	32 (19%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	160/170 (94%)	133 (83%)	27 (17%)	2 3
All	All	329/340 (97%)	270 (82%)	59 (18%)	2 2

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	9	LYS
1	A	17	THR
1	A	21	LEU
1	A	28	GLN
1	A	32	LEU
1	A	33	LEU
1	A	55	VAL
1	A	58	GLU
1	A	80	GLU
1	A	82	GLU
1	A	84	LEU
1	A	93	LEU
1	A	99	THR
1	A	103	LEU
1	A	108	LEU
1	A	120	ASN
1	A	122	ARG
1	A	135	SER
1	A	136	LYS
1	A	152	LEU
1	A	164	GLN
1	A	165	LYS
1	A	167	SER
1	A	168	LEU
1	A	172	VAL
1	A	174	SER
1	A	175	GLU
1	A	176	VAL
1	A	180	LYS
1	A	183	ILE
1	A	202	LEU
1	B	3	ILE
1	B	14	LYS
1	B	17	THR
1	B	21	LEU

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Mol	Chain	Res	Type
1	B	28	GLN
1	B	32	LEU
1	B	55	VAL
1	B	83	ASP
1	B	85	GLU
1	B	93	LEU
1	B	103	LEU
1	B	105	LEU
1	B	110	LEU
1	B	111	THR
1	B	113	GLU
1	B	120	ASN
1	B	129	ILE
1	B	130	ILE
1	B	133	TYR
1	B	167	SER
1	B	172	VAL
1	B	175	GLU
1	B	183	ILE
1	B	189	LYS
1	B	198	GLU
1	B	199	ILE
1	B	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	69	GLN
1	A	70	ASN
1	B	116	GLN
1	B	169	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)

2 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	ADP	B	301	-	24,29,29	1.33	3 (12%)	29,45,45	2.09	7 (24%)
2	ADP	A	301	-	24,29,29	0.99	2 (8%)	29,45,45	2.19	10 (34%)

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	ADP	B	301	-	-	0/12/32/32	0/3/3/3
2	ADP	A	301	-	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ADP	O4'-C1'	3.59	1.46	1.41
2	B	301	ADP	C5-C4	2.25	1.46	1.40
2	B	301	ADP	C4-N3	-2.17	1.32	1.35
2	A	301	ADP	PB-O3B	-2.14	1.46	1.54
2	A	301	ADP	O4'-C1'	2.01	1.43	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	ADP	O2B-PB-O3A	5.73	123.86	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	ADP	O3B-PB-O1B	-4.72	92.19	110.68
2	B	301	ADP	O3B-PB-O2B	4.41	124.47	107.64
2	B	301	ADP	C4-C5-N7	-4.31	104.91	109.40
2	A	301	ADP	N3-C2-N1	-3.87	122.62	128.68
2	B	301	ADP	PA-O3A-PB	-3.87	119.53	132.83
2	A	301	ADP	C4-C5-N7	-3.78	105.46	109.40
2	A	301	ADP	O3B-PB-O3A	-3.50	92.88	104.64
2	B	301	ADP	C5-C6-N6	2.86	124.69	120.35
2	A	301	ADP	C3'-C2'-C1'	2.85	105.27	100.98
2	A	301	ADP	O3B-PB-O2B	2.71	118.00	107.64
2	B	301	ADP	C5-C6-N1	-2.64	114.37	120.35
2	A	301	ADP	O2'-C2'-C1'	-2.36	102.12	110.85
2	A	301	ADP	C2'-C3'-C4'	2.24	106.99	102.64
2	B	301	ADP	O4'-C4'-C5'	-2.15	102.31	109.37
2	A	301	ADP	C5'-C4'-C3'	-2.13	107.20	115.18
2	A	301	ADP	O5'-PA-O1A	-2.02	101.17	109.07

There are no chirality outliers.

All (5) 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	A	301	ADP	O4'-C4'-C5'-O5'
2	A	301	ADP	C3'-C4'-C5'-O5'
2	A	301	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

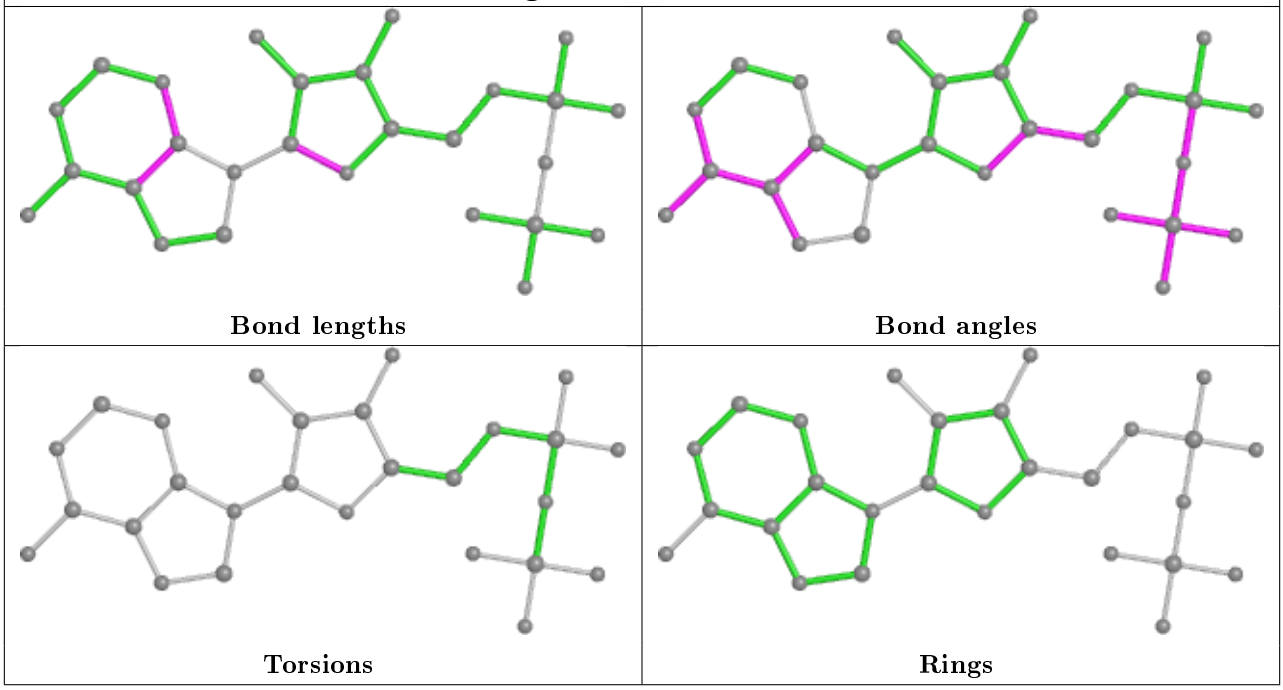
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ADP	1	0
2	A	301	ADP	5	0

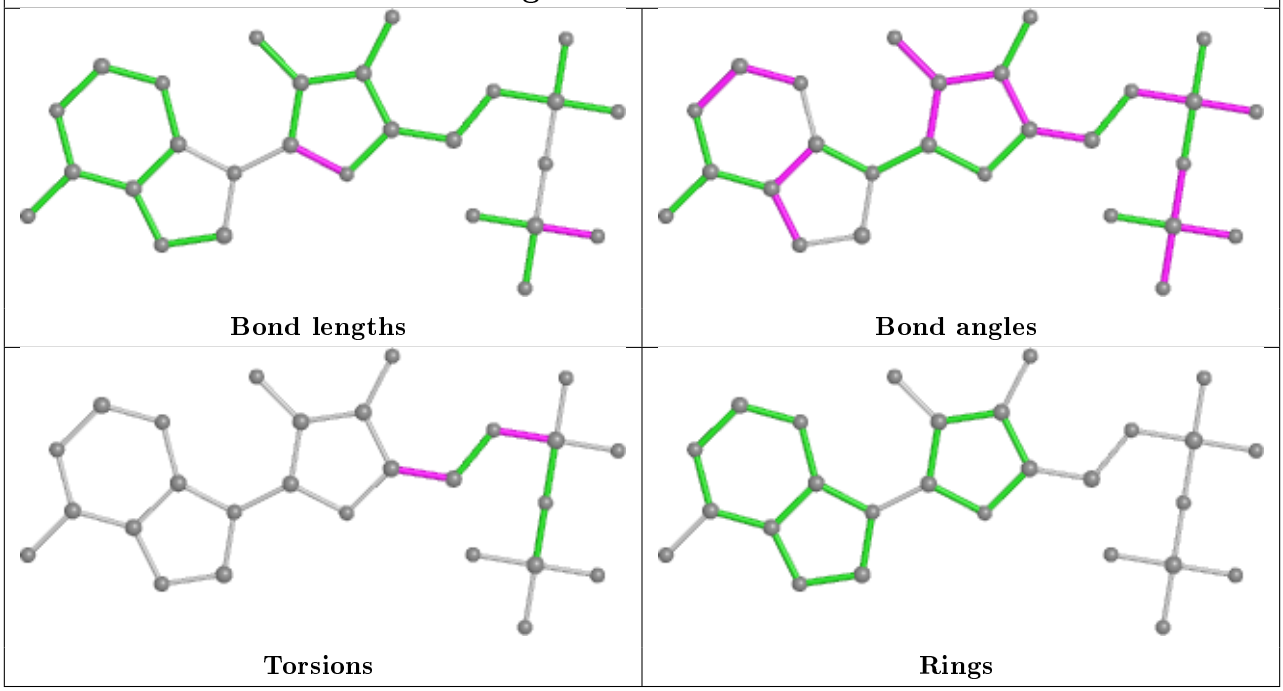
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 ADP B 301



Ligand ADP A 301



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	204/209 (97%)	0.08	7 (3%) 45 47	31, 44, 59, 82	0
1	B	195/209 (93%)	-0.09	3 (1%) 73 75	32, 42, 58, 77	0
All	All	399/418 (95%)	-0.01	10 (2%) 57 59	31, 43, 59, 82	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	TYR	5.5
1	A	21	LEU	3.1
1	B	17	THR	2.9
1	B	120	ASN	2.8
1	B	200	LEU	2.5
1	A	81	ASP	2.4
1	A	179	SER	2.4
1	A	177	SER	2.3
1	A	134	PRO	2.2
1	A	3	ILE	2.1

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 carbohydrates in this entry.

6.4 Ligands (i)

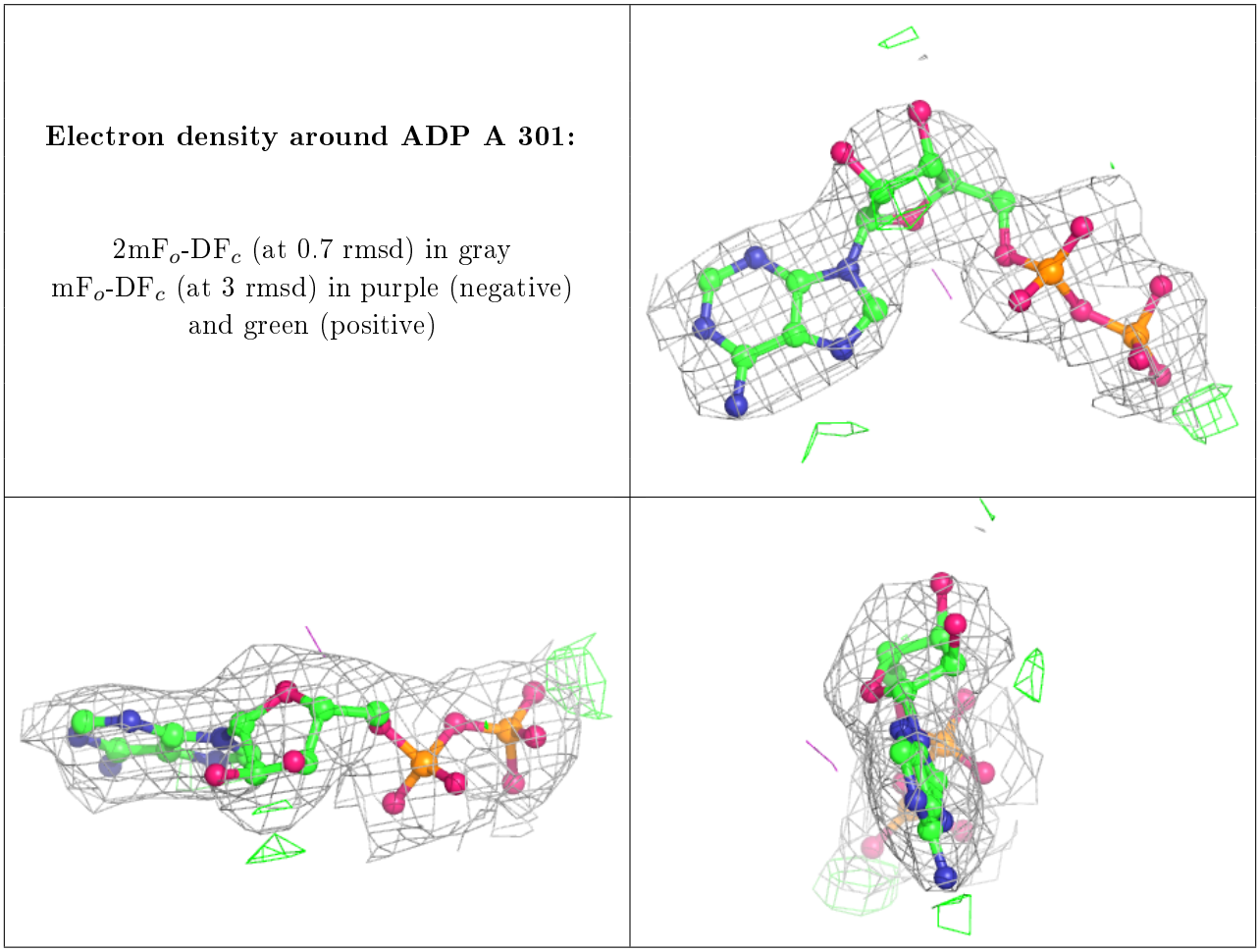
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ADP	A	301	27/27	0.96	0.14	39,43,53,56	0
2	ADP	B	301	27/27	0.98	0.12	33,40,47,54	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.

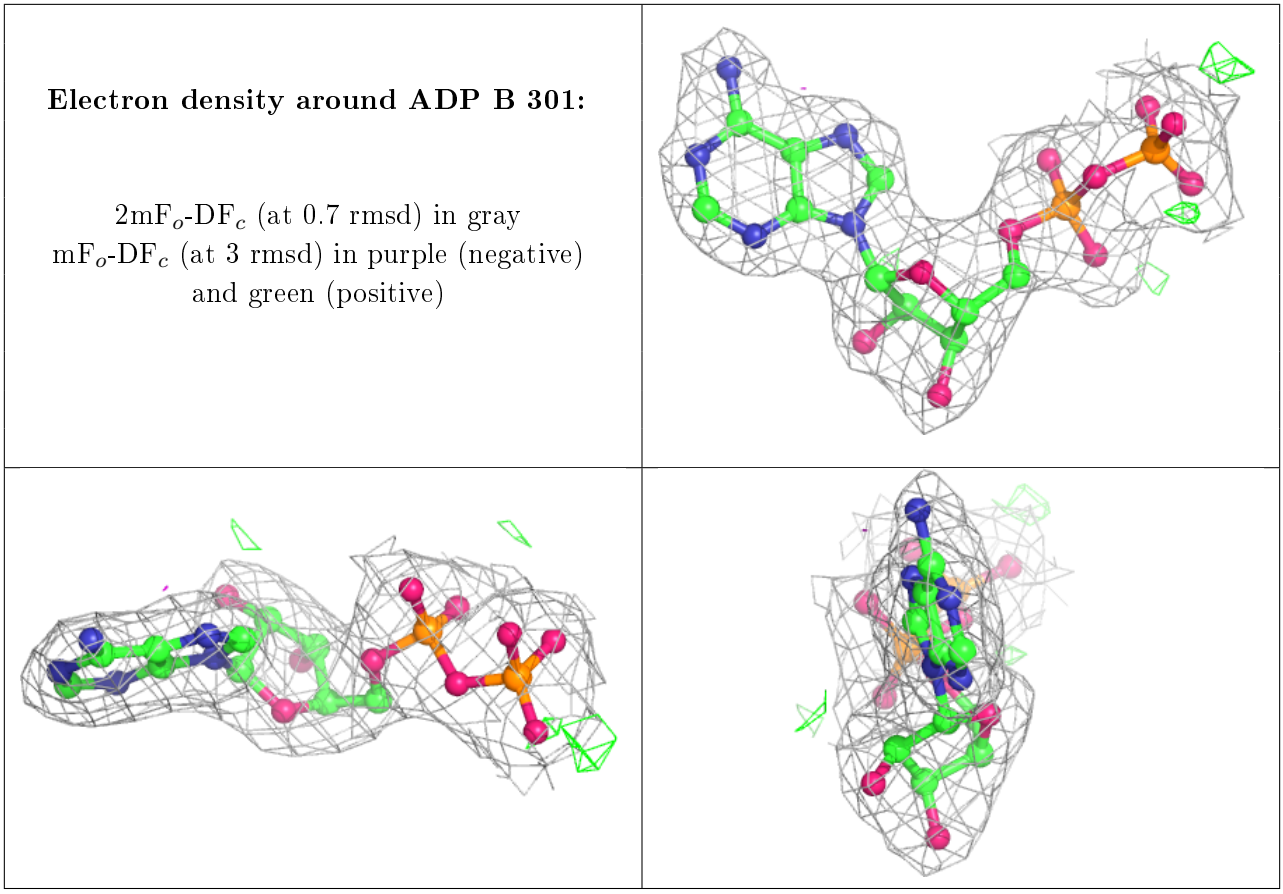
Electron density around ADP A 301:

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



Electron density around 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

There are no such residues in this entry.