



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:58 PM UTC

PDB ID : 2WE5 / pdb_00002we5
Title : Carbamate kinase from *Enterococcus faecalis* bound to MgADP
Authors : Ramon-Maiques, S.; Marina, A.; Rubio, V.
Deposited on : 2009-03-27
Resolution : 1.39 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

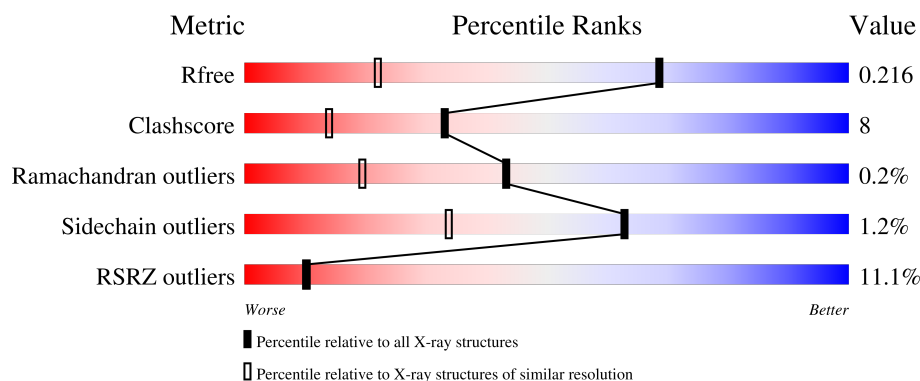
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	310	13% 86% 12%
1	B	310	9% 81% 18%
1	C	310	11% 82% 16%

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
4	ACT	A	1313	-	X	-	-

2 Entry composition [i](#)

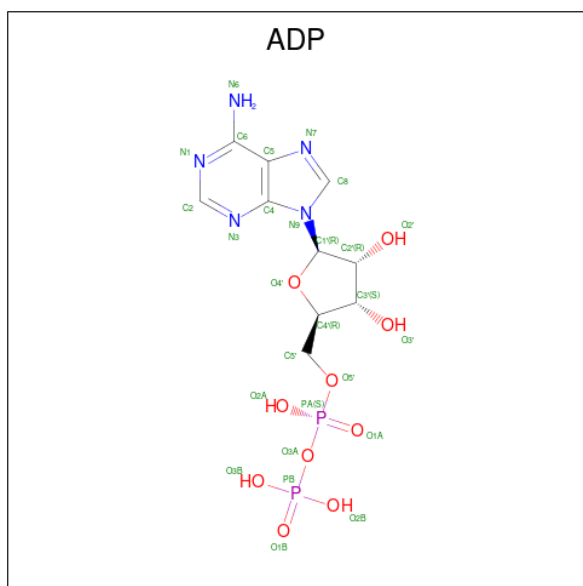
There are 5 unique types of molecules in this entry. The entry contains 8015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CARBAMATE KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	10	0
			2374	1497	401	467	9			
1	B	309	Total	C	N	O	S	0	6	0
			2347	1479	397	462	9			
1	C	309	Total	C	N	O	S	0	7	0
			2366	1487	404	466	9			

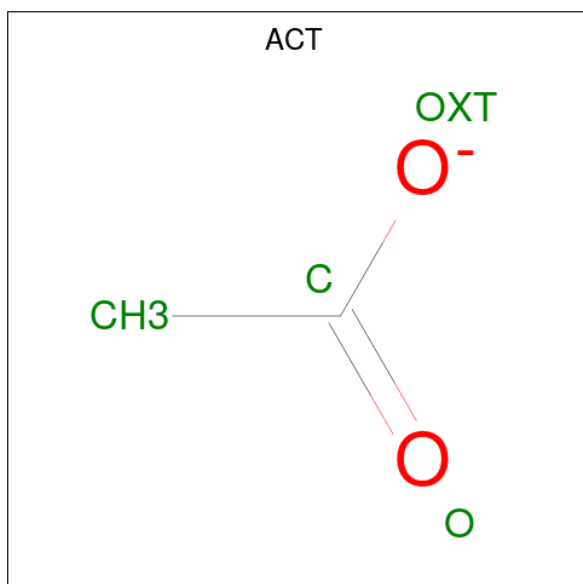
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

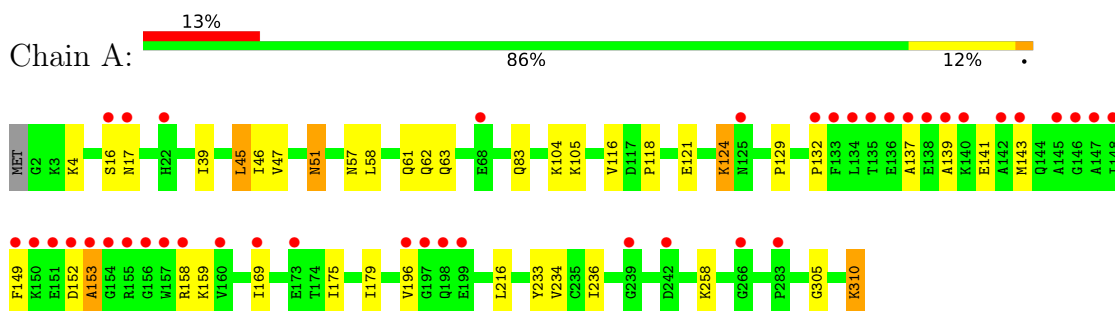
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total	O	0	0
			310	310		
5	B	282	Total	O	0	0
			282	282		
5	C	248	Total	O	0	0
			248	248		

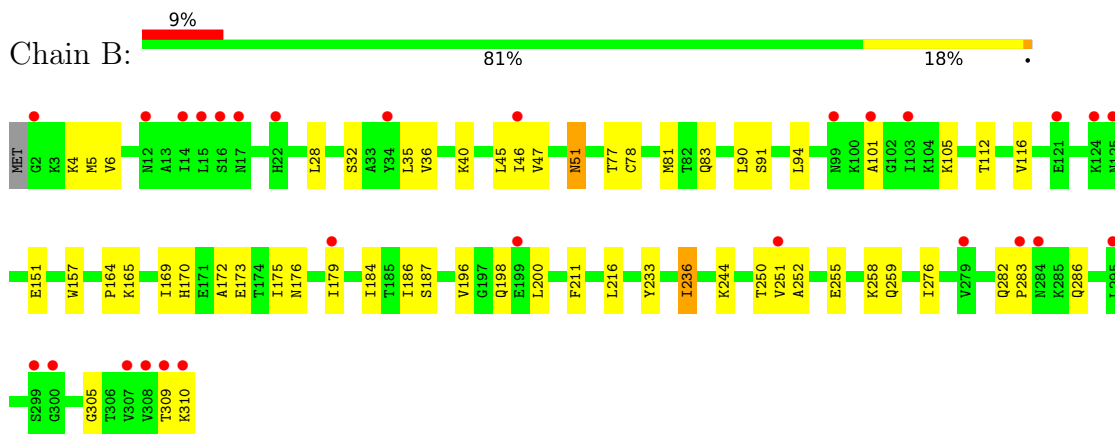
3 Residue-property plots

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.

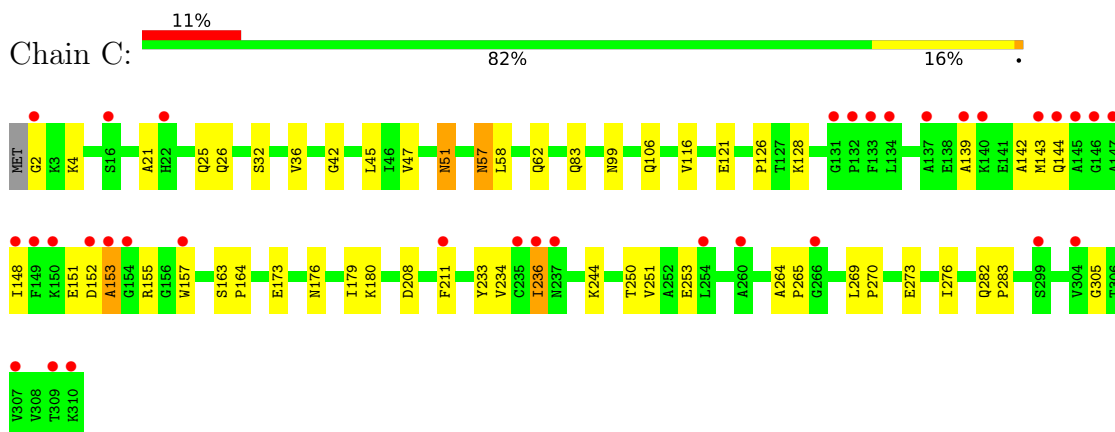
• Molecule 1: CARBAMATE KINASE 1



• Molecule 1: CARBAMATE KINASE 1



• Molecule 1: CARBAMATE KINASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.52Å 103.52Å 155.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.39 20.00 – 1.39	Depositor EDS
% Data completeness (in resolution range)	89.7 (20.00-1.39) 89.6 (20.00-1.39)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 1.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.210 0.206 , 0.216	Depositor DCC
R_{free} test set	8670 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8015	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ACT, 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	0.32	0/2410	0.84	6/3272 (0.2%)
1	B	0.31	0/2382	0.83	5/3231 (0.2%)
1	C	0.31	0/2401	0.82	5/3256 (0.2%)
All	All	0.32	0/7193	0.83	16/9759 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ILE	N-CA-C	-7.19	97.96	108.89
1	C	47	VAL	N-CA-C	6.78	118.82	108.71
1	A	234	VAL	N-CA-C	-6.60	101.02	109.80
1	A	47	VAL	N-CA-C	6.14	117.86	108.71
1	C	236	ILE	N-CA-C	-6.08	99.72	108.48
1	A	83	GLN	N-CA-C	-6.06	104.79	111.82
1	B	236	ILE	N-CA-C	-6.05	99.54	108.85
1	C	83	GLN	N-CA-C	-5.69	105.22	111.82
1	B	170	HIS	N-CA-C	5.63	117.86	111.11
1	B	45	LEU	N-CA-C	5.62	119.40	109.96
1	B	47	VAL	N-CA-C	5.58	117.62	108.97
1	B	83	GLN	N-CA-C	-5.49	105.45	111.82
1	A	4	LYS	N-CA-C	-5.26	100.59	108.96
1	C	45	LEU	N-CA-C	5.25	118.50	110.20
1	C	234	VAL	N-CA-C	-5.24	102.83	109.80
1	A	45	LEU	N-CA-C	5.20	118.69	109.96

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	2374	0	2411	35	0
1	B	2347	0	2383	46	0
1	C	2366	0	2395	35	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	3	0	0
5	A	310	0	0	4	0
5	B	282	0	0	3	0
5	C	248	0	0	1	0
All	All	8015	0	7228	112	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 8.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:HA	1:B:46:ILE:HG23	1.47	0.95
1:B:112[B]:THR:HG21	1:B:187:SER:HB2	1.64	0.79
1:C:151:GLU:HG2	1:C:153:ALA:H	1.49	0.75
1:C:4:LYS:HE3	1:C:179:ILE:HG21	1.69	0.75
1:A:175:ILE:O	1:A:179[A]:ILE:HG12	1.88	0.74
1:B:46:ILE:HD12	1:B:179:ILE:HD11	1.70	0.73
1:B:35:LEU:HD12	1:B:94[B]:LEU:HD21	1.71	0.72
1:B:236:ILE:HD11	1:B:244:LYS:HD3	1.73	0.69
1:B:255:GLU:O	1:B:259:GLN:HG2	1.93	0.69
1:B:78:CYS:HA	1:B:81:MET:HE3	1.74	0.68
1:A:137:ALA:O	1:A:141:GLU:HG2	1.94	0.67
1:C:152:ASP:OD2	1:C:155:ARG:HD3	1.95	0.66
1:A:46:ILE:HG12	1:A:179[A]:ILE:HD12	1.77	0.66
1:B:77:THR:HG22	1:B:81:MET:HE2	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:GLY:HA2	1:C:42:GLY:O	1.97	0.65
1:B:46:ILE:HD11	1:B:216:LEU:HD21	1.80	0.64
1:B:198:GLN:HE21	1:C:99:ASN:HB3	1.62	0.64
1:C:236:ILE:HD11	1:C:244:LYS:HD3	1.80	0.63
1:C:176[A]:ASN:ND2	1:C:180:LYS:HE3	2.13	0.63
1:B:4:LYS:HE3	1:B:179:ILE:HG21	1.82	0.62
1:B:252:ALA:H	1:B:310:LYS:NZ	1.99	0.60
1:C:173[A]:GLU:HG3	5:C:2146:HOH:O	2.02	0.60
1:A:118:PRO:HB3	1:A:196[B]:VAL:HG11	1.83	0.59
1:B:91[B]:SER:OG	1:B:186:ILE:HD12	2.03	0.58
1:B:309:THR:O	1:B:310:LYS:HB2	2.03	0.58
1:C:233:TYR:CE2	1:C:305:GLY:HA2	2.41	0.56
1:C:116:VAL:HG11	1:C:164:PRO:HG2	1.86	0.56
1:A:63[B]:GLN:CD	1:A:132:PRO:HG3	2.31	0.56
1:B:200:LEU:HD12	5:B:2110:HOH:O	2.07	0.55
1:C:21:ALA:O	1:C:25:GLN:HG3	2.07	0.55
1:B:250:THR:HB	1:B:310:LYS:HD3	1.87	0.55
1:B:165:LYS:HE2	1:B:211:PHE:CE1	2.43	0.54
1:A:104:LYS:NZ	1:C:106:GLN:HG2	2.23	0.54
1:A:179[A]:ILE:HD13	5:A:2067:HOH:O	2.07	0.54
1:A:46:ILE:HG12	1:A:179[A]:ILE:CD1	2.39	0.53
1:B:233:TYR:CE2	1:B:305:GLY:HA2	2.45	0.52
1:A:233:TYR:CE2	1:A:305:GLY:HA2	2.45	0.52
1:A:310:LYS:O	1:A:310:LYS:HE3	2.09	0.51
1:A:124:LYS:NZ	1:A:124:LYS:HB3	2.26	0.51
1:B:32:SER:O	1:B:36:VAL:HG23	2.10	0.51
1:A:51:ASN:ND2	1:A:51:ASN:C	2.69	0.50
1:C:269:LEU:HB3	1:C:270:PRO:HD3	1.92	0.50
1:A:152:ASP:O	1:A:153:ALA:C	2.55	0.50
1:A:310:LYS:HG3	5:A:2137:HOH:O	2.10	0.50
1:C:251:VAL:HG13	1:C:276:ILE:HG23	1.93	0.49
1:A:116:VAL:HG23	1:A:196[A]:VAL:HG12	1.94	0.49
1:C:269:LEU:O	1:C:273:GLU:HG3	2.12	0.49
1:B:173:GLU:HB3	5:B:2188:HOH:O	2.11	0.49
1:C:250:THR:OG1	1:C:253:GLU:HG3	2.13	0.49
1:B:252:ALA:CB	1:B:310:LYS:HZ1	2.26	0.48
1:A:118:PRO:HD3	1:A:196[B]:VAL:HG13	1.95	0.48
1:B:116:VAL:HG11	1:B:164:PRO:HG2	1.96	0.48
1:B:175:ILE:O	1:B:179:ILE:HG13	2.13	0.48
1:A:104:LYS:HZ3	1:C:106:GLN:HG2	1.77	0.47
1:A:16:SER:O	1:A:17:ASN:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ALA:O	1:C:143:MET:HG3	2.14	0.47
1:B:5:MET:O	1:B:46:ILE:HG22	2.15	0.47
1:C:26:GLN:NE2	1:C:26:GLN:HA	2.30	0.47
1:C:208:ASP:HB3	1:C:211:PHE:CD2	2.50	0.46
1:C:128:LYS:HG2	1:C:163:SER:HB2	1.96	0.46
1:B:112[B]:THR:CG2	1:B:187:SER:HB2	2.42	0.46
1:B:198:GLN:NE2	1:C:99:ASN:HB3	2.30	0.46
1:B:51:ASN:ND2	1:B:51:ASN:C	2.72	0.46
1:C:176[A]:ASN:HD21	1:C:180:LYS:HE3	1.80	0.45
1:B:258:LYS:NZ	1:B:259:GLN:HE22	2.14	0.45
1:A:121:GLU:O	1:A:124:LYS:HG2	2.15	0.45
1:C:51:ASN:C	1:C:51:ASN:ND2	2.74	0.45
1:A:169[B]:ILE:HD12	1:A:216:LEU:HA	1.99	0.45
1:C:142:ALA:C	1:C:144:GLN:H	2.23	0.45
1:A:39:ILE:HD11	1:A:45:LEU:HG	1.98	0.45
1:B:6:VAL:CA	1:B:46:ILE:HG23	2.34	0.45
1:C:51:ASN:HD22	1:C:51:ASN:N	2.14	0.45
1:C:57:ASN:HD22	1:C:57:ASN:HA	1.59	0.45
1:B:28:LEU:HD22	1:B:90:LEU:HD13	1.98	0.44
1:A:258:LYS:C	1:A:258:LYS:HD3	2.42	0.44
1:B:151:GLU:HB2	1:B:157:TRP:CE2	2.52	0.44
1:C:282:GLN:HB3	1:C:283:PRO:HD2	1.99	0.44
1:A:51:ASN:C	1:A:51:ASN:HD22	2.23	0.44
1:B:116:VAL:HG23	1:B:196:VAL:HG12	2.00	0.44
1:B:46:ILE:HD11	1:B:216:LEU:CD2	2.48	0.43
1:B:251:VAL:HG13	1:B:276:ILE:HG23	2.00	0.43
1:B:252:ALA:H	1:B:310:LYS:HZ1	1.65	0.43
1:A:129:PRO:HB2	1:A:158:ARG:HD3	2.00	0.43
1:A:58:LEU:O	1:A:62:GLN:HG2	2.18	0.43
1:C:58:LEU:O	1:C:62:GLN:HG2	2.19	0.43
1:C:121:GLU:CD	1:C:121:GLU:C	2.87	0.43
1:C:264:ALA:HA	1:C:265:PRO:HD3	1.93	0.42
1:B:46:ILE:HG13	5:B:2196:HOH:O	2.20	0.42
1:A:175:ILE:O	1:A:179[B]:ILE:HG13	2.20	0.42
1:A:179[A]:ILE:CD1	5:A:2067:HOH:O	2.66	0.42
1:B:40:LYS:HE2	1:B:101:ALA:HB1	2.01	0.42
1:B:258:LYS:NZ	1:B:259:GLN:NE2	2.68	0.42
1:B:252:ALA:HB2	1:B:310:LYS:HZ1	1.84	0.42
1:B:282:GLN:HG2	1:B:283:PRO:HD2	2.02	0.42
1:C:126:PRO:HG3	1:C:148:ILE:HD12	2.02	0.42
1:A:139:ALA:O	1:A:143:MET:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:PHE:CZ	1:A:159:LYS:HB2	2.55	0.41
1:B:236:ILE:CG1	1:B:244:LYS:HB3	2.50	0.41
1:B:51:ASN:N	1:B:51:ASN:HD22	2.18	0.41
1:A:51:ASN:HD22	1:A:51:ASN:N	2.18	0.41
1:A:121:GLU:HG2	5:A:2159:HOH:O	2.20	0.41
1:C:151:GLU:HB2	1:C:157:TRP:CE2	2.56	0.41
1:C:32:SER:O	1:C:36:VAL:HG23	2.21	0.41
1:C:51:ASN:C	1:C:51:ASN:HD22	2.29	0.41
1:A:57:ASN:O	1:A:61:GLN:HG3	2.21	0.41
1:B:46:ILE:HG23	1:B:46:ILE:O	2.21	0.41
1:B:6:VAL:HG22	1:B:46:ILE:CG2	2.52	0.40
1:B:169[A]:ILE:HB	1:B:172:ALA:HB2	2.03	0.40
1:A:51:ASN:HD22	1:A:51:ASN:H	1.69	0.40
1:A:63[A]:GLN:HG3	1:A:132:PRO:HG3	2.03	0.40
1:B:105:LYS:HG2	1:B:184:ILE:CD1	2.52	0.40
1:A:118:PRO:HD3	1:A:196[B]:VAL:CG1	2.52	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	317/310 (102%)	307 (97%)	9 (3%)	1 (0%)	36	16
1	B	313/310 (101%)	305 (97%)	8 (3%)	0	100	100
1	C	314/310 (101%)	304 (97%)	9 (3%)	1 (0%)	36	16
All	All	944/930 (102%)	916 (97%)	26 (3%)	2 (0%)	43	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	153	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/249 (104%)	254 (98%)	4 (2%)	55	23
1	B	254/249 (102%)	251 (99%)	3 (1%)	63	34
1	C	255/249 (102%)	253 (99%)	2 (1%)	73	48
All	All	767/747 (103%)	758 (99%)	9 (1%)	63	34

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	105	LYS
1	A	124	LYS
1	A	310	LYS
1	B	51	ASN
1	B	176	ASN
1	B	286	GLN
1	C	51	ASN
1	C	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	41	GLN
1	A	51	ASN
1	A	92	ASN
1	A	96	GLN
1	A	99	ASN
1	A	113	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	ASN
1	A	277	GLN
1	B	17	ASN
1	B	22	HIS
1	B	25	GLN
1	B	51	ASN
1	B	92	ASN
1	B	99	ASN
1	B	113	GLN
1	B	176	ASN
1	B	198	GLN
1	B	259	GLN
1	B	277	GLN
1	B	282	GLN
1	C	25	GLN
1	C	26	GLN
1	C	41	GLN
1	C	51	ASN
1	C	57	ASN
1	C	113	GLN
1	C	144	GLN
1	C	237	ASN
1	C	248	ASN
1	C	282	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
2	ADP	A	1311	3	28,29,29	1.61	6 (21%)	43,45,45	1.49	9 (20%)
2	ADP	B	1311	3	28,29,29	1.61	6 (21%)	43,45,45	1.47	7 (16%)
4	ACT	A	1313	-	3,3,3	1.47	1 (33%)	3,3,3	2.82	2 (66%)
2	ADP	C	1311	3	28,29,29	1.66	5 (17%)	43,45,45	1.50	10 (23%)

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	A	1311	3	-	7/16/32/32	0/3/3/3
2	ADP	B	1311	3	-	6/16/32/32	0/3/3/3
2	ADP	C	1311	3	-	6/16/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1311	ADP	C2-N1	4.26	1.41	1.33
2	A	1311	ADP	C2-N1	4.08	1.41	1.33
2	B	1311	ADP	C2-N1	4.00	1.41	1.33
2	C	1311	ADP	C4-N3	3.46	1.40	1.34
2	A	1311	ADP	C4-N3	3.41	1.40	1.34
2	B	1311	ADP	C4-N3	3.40	1.40	1.34
2	A	1311	ADP	C5-N7	-2.53	1.34	1.39
2	C	1311	ADP	C5-N7	-2.51	1.34	1.39
2	B	1311	ADP	C5-N7	-2.46	1.34	1.39
4	A	1313	ACT	O-C	2.36	1.32	1.22
2	B	1311	ADP	O2'-C2'	2.29	1.48	1.43
2	C	1311	ADP	O2'-C2'	2.26	1.48	1.43
2	B	1311	ADP	C3'-C4'	-2.18	1.47	1.53
2	A	1311	ADP	O4'-C1'	2.07	1.46	1.42
2	A	1311	ADP	O2'-C2'	2.05	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1311	ADP	O4'-C1'	2.04	1.46	1.42
2	B	1311	ADP	O4'-C1'	2.04	1.46	1.42
2	A	1311	ADP	PA-O2A	-2.03	1.45	1.55

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1311	ADP	C4'-O4'-C1'	-4.05	100.52	109.47
2	C	1311	ADP	C4'-O4'-C1'	-3.94	100.78	109.47
2	A	1311	ADP	C4'-O4'-C1'	-3.91	100.83	109.47
4	A	1313	ACT	O-C-CH3	-3.91	106.51	122.53
2	A	1311	ADP	N6-C6-N1	-3.32	110.99	118.38
2	C	1311	ADP	N6-C6-N1	-3.22	111.20	118.38
2	B	1311	ADP	O4'-C1'-N9	-3.19	101.96	108.09
2	B	1311	ADP	N6-C6-N1	-3.13	111.39	118.38
2	C	1311	ADP	O4'-C1'-N9	-3.06	102.22	108.09
2	A	1311	ADP	O4'-C1'-N9	-2.93	102.47	108.09
2	A	1311	ADP	C5-C6-N6	2.80	130.22	123.29
2	C	1311	ADP	C5-C6-N6	2.76	130.12	123.29
2	B	1311	ADP	C5-C6-N6	2.63	129.80	123.29
2	C	1311	ADP	C4-N9-C1'	2.54	132.56	126.63
2	A	1311	ADP	C4-N9-C1'	2.53	132.55	126.63
2	B	1311	ADP	C4-N9-C1'	2.49	132.46	126.63
4	A	1313	ACT	OXT-C-CH3	2.35	124.91	115.05
2	A	1311	ADP	O3'-C3'-C2'	2.26	119.07	111.82
2	C	1311	ADP	O3'-C3'-C2'	2.25	119.03	111.82
2	B	1311	ADP	O3'-C3'-C2'	2.18	118.81	111.82
2	B	1311	ADP	N3-C2-N1	-2.18	125.28	128.58
2	A	1311	ADP	O3B-PB-O3A	2.17	111.91	104.64
2	C	1311	ADP	N3-C2-N1	-2.14	125.34	128.58
2	A	1311	ADP	N3-C2-N1	-2.05	125.48	128.58
2	C	1311	ADP	O3B-PB-O3A	2.03	111.44	104.64
2	C	1311	ADP	O2A-PA-O3A	2.02	112.75	107.27
2	C	1311	ADP	O3'-C3'-C4'	2.02	116.88	111.08
2	A	1311	ADP	C4-N9-C8	-2.00	103.64	105.74

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1311	ADP	C4'-C5'-O5'-PA
2	B	1311	ADP	C2'-C1'-N9-C4

Continued on next page...

Continued from previous page...

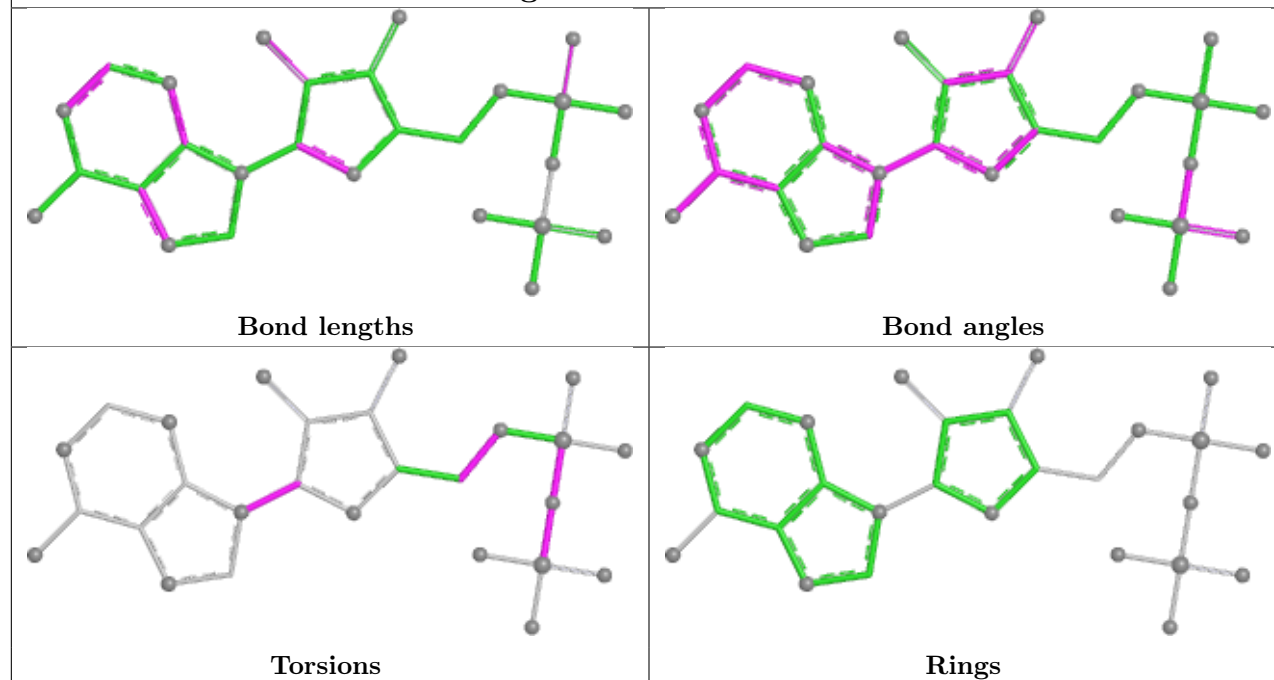
Mol	Chain	Res	Type	Atoms
2	A	1311	ADP	C4'-C5'-O5'-PA
2	C	1311	ADP	C4'-C5'-O5'-PA
2	A	1311	ADP	PB-O3A-PA-O2A
2	B	1311	ADP	PB-O3A-PA-O2A
2	C	1311	ADP	PB-O3A-PA-O2A
2	B	1311	ADP	C2'-C1'-N9-C8
2	A	1311	ADP	C2'-C1'-N9-C8
2	A	1311	ADP	C2'-C1'-N9-C4
2	C	1311	ADP	C2'-C1'-N9-C4
2	C	1311	ADP	C2'-C1'-N9-C8
2	A	1311	ADP	PA-O3A-PB-O2B
2	C	1311	ADP	O4'-C1'-N9-C8
2	A	1311	ADP	O4'-C1'-N9-C8
2	B	1311	ADP	O4'-C1'-N9-C8
2	A	1311	ADP	PB-O3A-PA-O1A
2	B	1311	ADP	PB-O3A-PA-O1A
2	C	1311	ADP	PB-O3A-PA-O1A

There are no ring outliers.

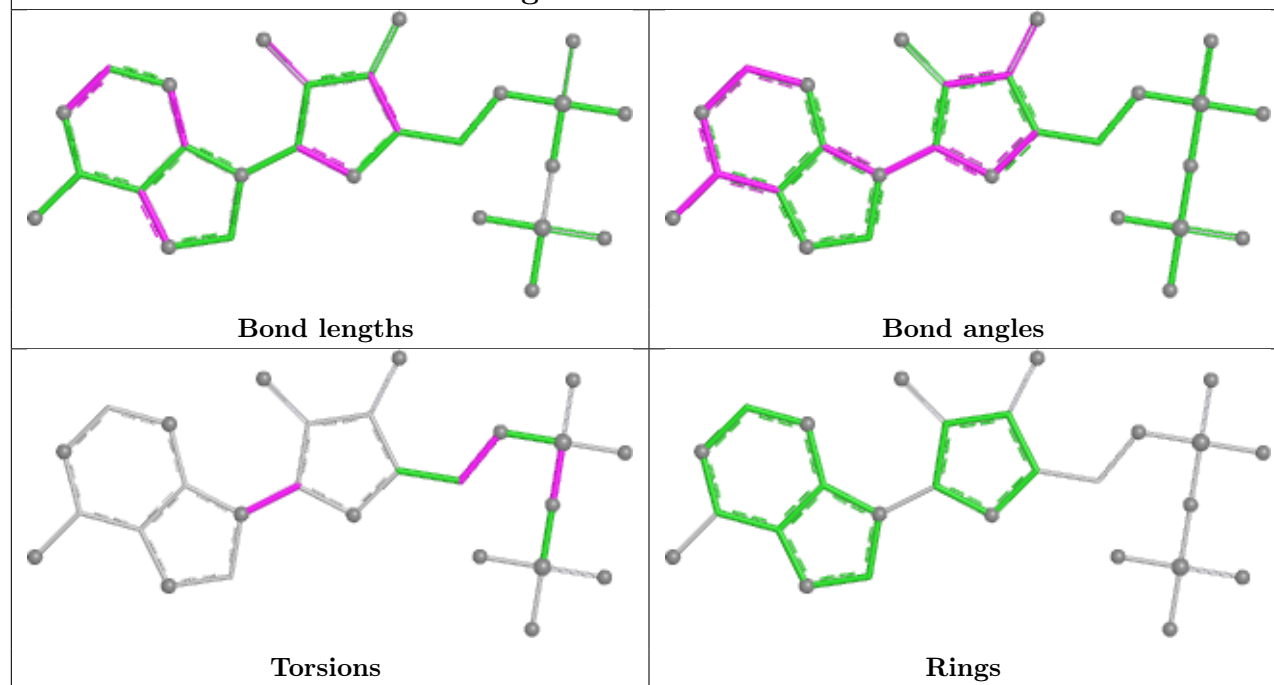
No monomer is involved in short contacts.

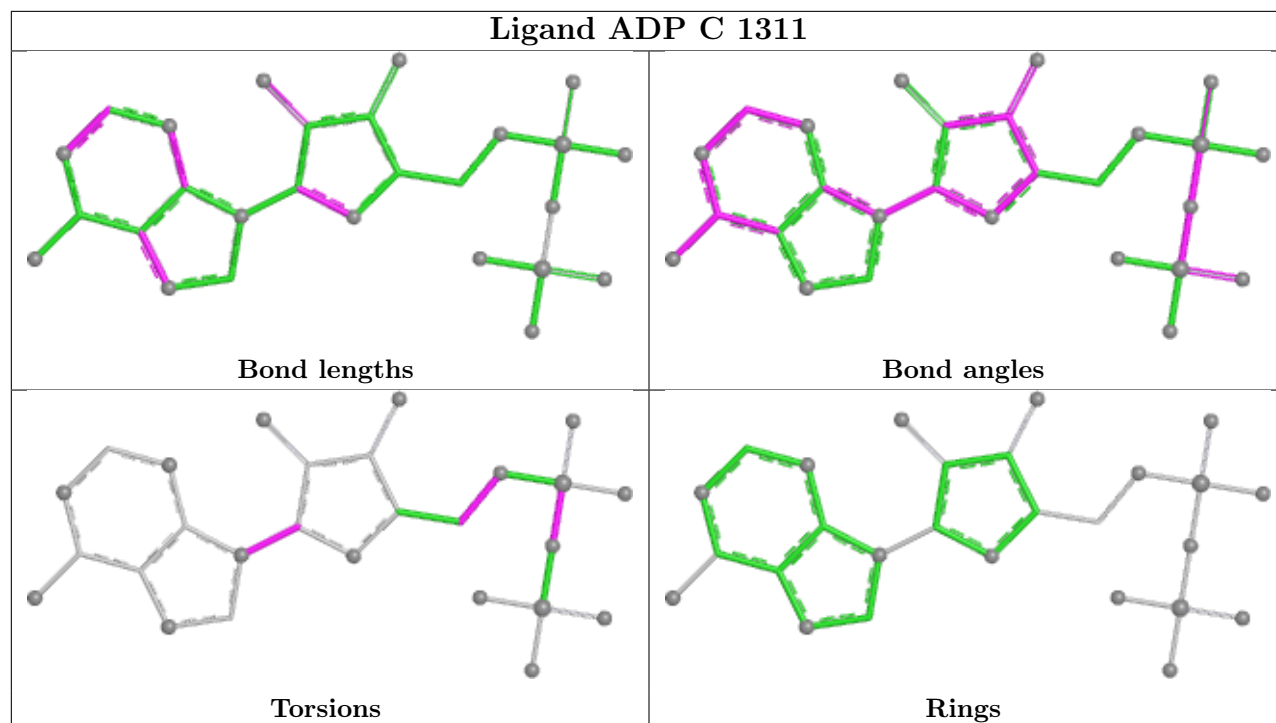
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ADP A 1311



Ligand ADP B 1311





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	309/310 (99%)	0.71	41 (13%) 7 7	8, 19, 45, 65	10 (3%)
1	B	309/310 (99%)	0.72	28 (9%) 15 14	8, 21, 36, 42	6 (1%)
1	C	309/310 (99%)	0.89	34 (11%) 10 10	11, 22, 46, 63	7 (2%)
All	All	927/930 (99%)	0.77	103 (11%) 10 10	8, 21, 39, 65	23 (2%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	TRP	8.1
1	A	153	ALA	7.8
1	A	137	ALA	5.5
1	A	17	ASN	5.3
1	B	15	LEU	4.9
1	A	135	THR	4.8
1	C	153	ALA	4.8
1	B	46	ILE	4.7
1	C	154	GLY	4.6
1	A	134	LEU	4.6
1	C	149	PHE	4.5
1	C	133	PHE	4.5
1	C	148	ILE	4.4
1	A	151	GLU	4.4
1	C	147	ALA	4.3
1	A	266	GLY	4.2
1	A	149	PHE	4.2
1	A	139	ALA	4.2
1	A	198	GLN	4.2
1	C	150[A]	LYS	4.1
1	C	157	TRP	4.0
1	A	154	GLY	3.9
1	C	2	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	16	SER	3.8
1	C	139	ALA	3.7
1	C	309	THR	3.7
1	C	143	MET	3.6
1	B	310	LYS	3.6
1	B	2	GLY	3.5
1	A	132	PRO	3.5
1	A	156	GLY	3.5
1	C	152	ASP	3.4
1	A	152	ASP	3.4
1	A	146	GLY	3.4
1	A	197	GLY	3.4
1	A	136	GLU	3.3
1	A	160[A]	VAL	3.3
1	A	133	PHE	3.2
1	C	16	SER	3.2
1	C	137	ALA	3.1
1	C	140	LYS	3.1
1	A	199	GLU	3.1
1	C	146	GLY	3.0
1	B	309	THR	2.9
1	C	145	ALA	2.9
1	B	22	HIS	2.9
1	A	169[A]	ILE	2.8
1	A	140	LYS	2.8
1	C	260	ALA	2.8
1	A	148	ILE	2.8
1	A	143	MET	2.7
1	C	304	VAL	2.7
1	A	196[A]	VAL	2.7
1	B	14	ILE	2.7
1	B	17	ASN	2.7
1	B	125	ASN	2.7
1	A	150	LYS	2.6
1	B	179	ILE	2.6
1	C	266	GLY	2.6
1	C	134	LEU	2.6
1	C	211	PHE	2.6
1	B	16	SER	2.6
1	C	236	ILE	2.6
1	B	308	VAL	2.5
1	A	155	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	125	ASN	2.5
1	B	121	GLU	2.5
1	B	299	SER	2.5
1	A	145	ALA	2.5
1	A	147	ALA	2.5
1	B	283	PRO	2.4
1	B	307	VAL	2.4
1	B	199	GLU	2.4
1	C	22	HIS	2.4
1	C	132	PRO	2.4
1	B	34	TYR	2.4
1	A	158	ARG	2.3
1	A	283	PRO	2.3
1	A	68	GLU	2.3
1	A	138	GLU	2.3
1	A	22	HIS	2.3
1	B	99	ASN	2.3
1	B	251	VAL	2.3
1	C	310	LYS	2.3
1	B	284	ASN	2.3
1	C	144	GLN	2.3
1	B	124[A]	LYS	2.3
1	C	307	VAL	2.3
1	C	235	CYS	2.2
1	A	239	GLY	2.2
1	B	300	GLY	2.2
1	B	295	LEU	2.2
1	B	103	ILE	2.2
1	B	279	VAL	2.2
1	A	142	ALA	2.2
1	A	242	ASP	2.2
1	C	299	SER	2.2
1	C	237	ASN	2.1
1	A	173	GLU	2.1
1	C	254	LEU	2.1
1	C	131	GLY	2.1
1	B	101	ALA	2.1
1	B	12	ASN	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

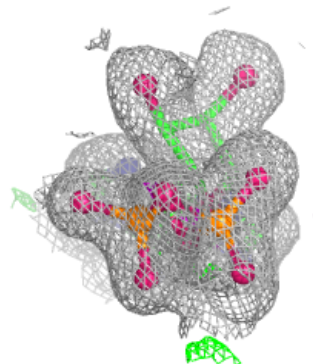
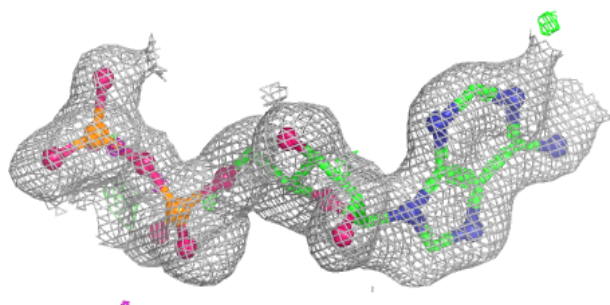
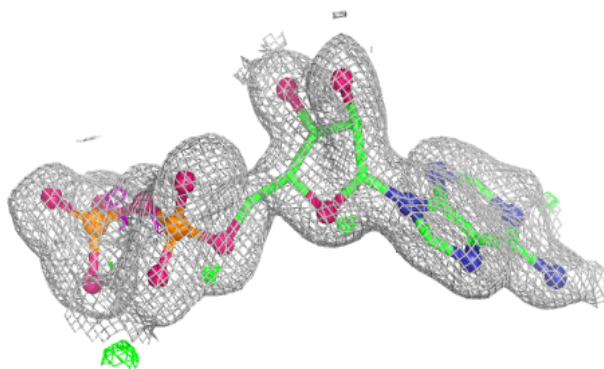
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	1313	4/4	0.91	0.09	22,27,27,28	0
3	MG	C	1312	1/1	0.92	0.07	24,24,24,24	0
2	ADP	C	1311	27/27	0.96	0.07	21,23,26,29	0
2	ADP	B	1311	27/27	0.98	0.05	16,18,20,20	0
2	ADP	A	1311	27/27	0.98	0.04	15,17,18,21	0
3	MG	A	1312	1/1	0.99	0.05	16,16,16,16	0
3	MG	B	1312	1/1	0.99	0.02	18,18,18,18	0

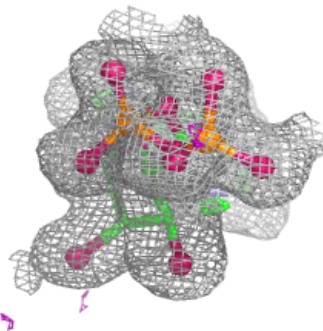
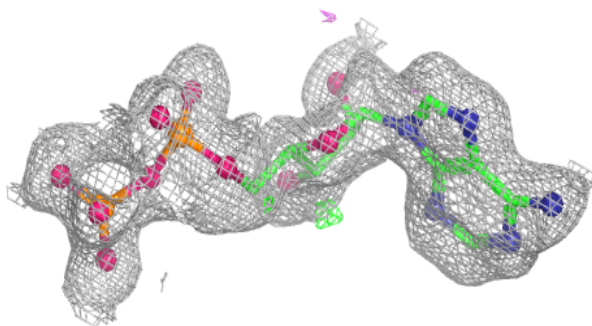
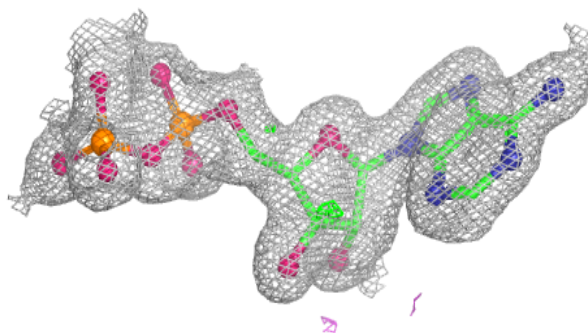
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

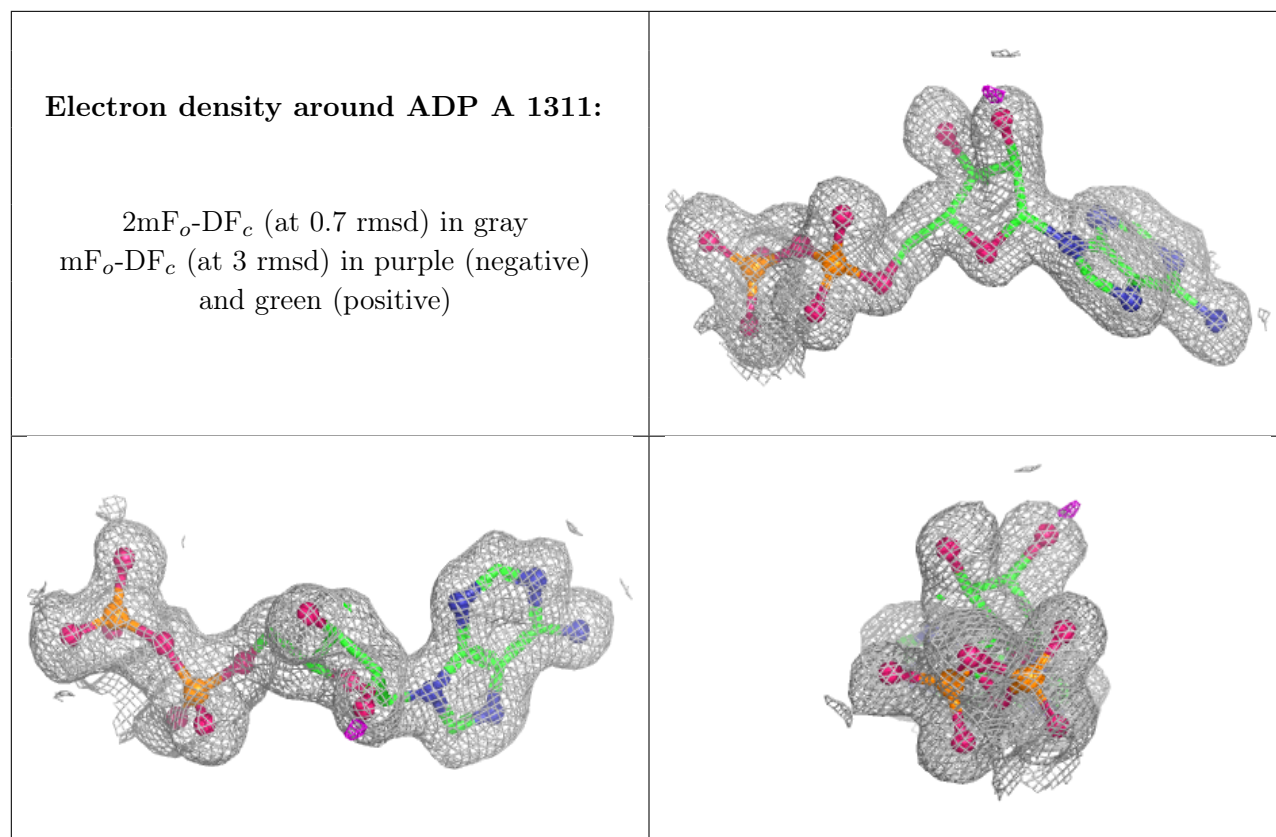
Electron density around ADP C 1311:

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

**Electron density around ADP B 1311:**

$2mF_o-DF_c$ (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.