Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 05:52 PM JST

PDB ID	:	5Y0Q
Title	:	Crystal structure of BsTmcAL bound with AMPCPP
Authors	:	Yamashita, S.; Tomita, K.
Deposited on	:	2017-07-18
Resolution	:	2.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

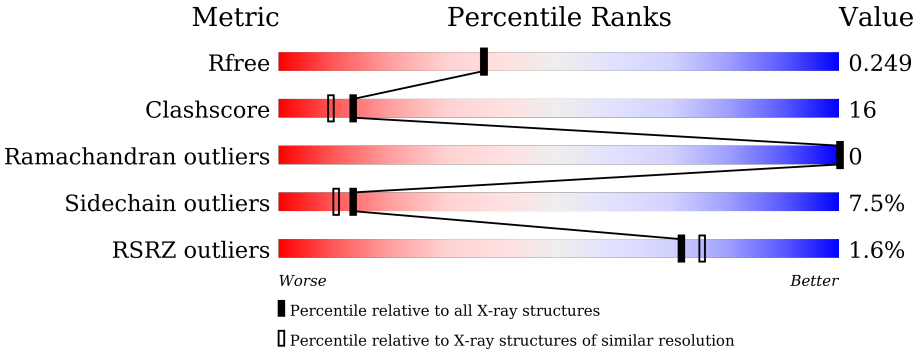
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	434	2% 59% 30% • 8%
1	B	434	.% 59% 30% • 8%

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	APC	A	1001	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6539 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 UPF0348 protein B4417_3650.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3205	2047	553	593	12	0	0	0
1	B	401	3205	2047	553	593	12	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP A0A164SIT4
A	-17	GLY	-	expression tag	UNP A0A164SIT4
A	-16	SER	-	expression tag	UNP A0A164SIT4
A	-15	SER	-	expression tag	UNP A0A164SIT4
A	-14	HIS	-	expression tag	UNP A0A164SIT4
A	-13	HIS	-	expression tag	UNP A0A164SIT4
A	-12	HIS	-	expression tag	UNP A0A164SIT4
A	-11	HIS	-	expression tag	UNP A0A164SIT4
A	-10	HIS	-	expression tag	UNP A0A164SIT4
A	-9	HIS	-	expression tag	UNP A0A164SIT4
A	-8	SER	-	expression tag	UNP A0A164SIT4
A	-7	SER	-	expression tag	UNP A0A164SIT4
A	-6	GLY	-	expression tag	UNP A0A164SIT4
A	-5	LEU	-	expression tag	UNP A0A164SIT4
A	-4	VAL	-	expression tag	UNP A0A164SIT4
A	-3	PRO	-	expression tag	UNP A0A164SIT4
A	-2	ARG	-	expression tag	UNP A0A164SIT4
A	-1	GLY	-	expression tag	UNP A0A164SIT4
A	0	SER	-	expression tag	UNP A0A164SIT4
B	-18	MET	-	expression tag	UNP A0A164SIT4
B	-17	GLY	-	expression tag	UNP A0A164SIT4
B	-16	SER	-	expression tag	UNP A0A164SIT4
B	-15	SER	-	expression tag	UNP A0A164SIT4
B	-14	HIS	-	expression tag	UNP A0A164SIT4
B	-13	HIS	-	expression tag	UNP A0A164SIT4

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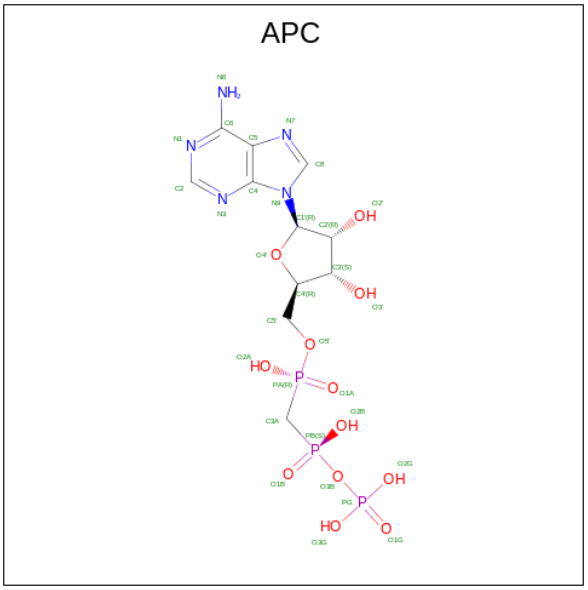
Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A164SIT4
B	-11	HIS	-	expression tag	UNP A0A164SIT4
B	-10	HIS	-	expression tag	UNP A0A164SIT4
B	-9	HIS	-	expression tag	UNP A0A164SIT4
B	-8	SER	-	expression tag	UNP A0A164SIT4
B	-7	SER	-	expression tag	UNP A0A164SIT4
B	-6	GLY	-	expression tag	UNP A0A164SIT4
B	-5	LEU	-	expression tag	UNP A0A164SIT4
B	-4	VAL	-	expression tag	UNP A0A164SIT4
B	-3	PRO	-	expression tag	UNP A0A164SIT4
B	-2	ARG	-	expression tag	UNP A0A164SIT4
B	-1	GLY	-	expression tag	UNP A0A164SIT4
B	0	SER	-	expression tag	UNP A0A164SIT4

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	11	5	12	3	0	0
			Total	C	N	O	P		
2	B	1	31	11	5	12	3	0	0

- Molecule 3 is water.

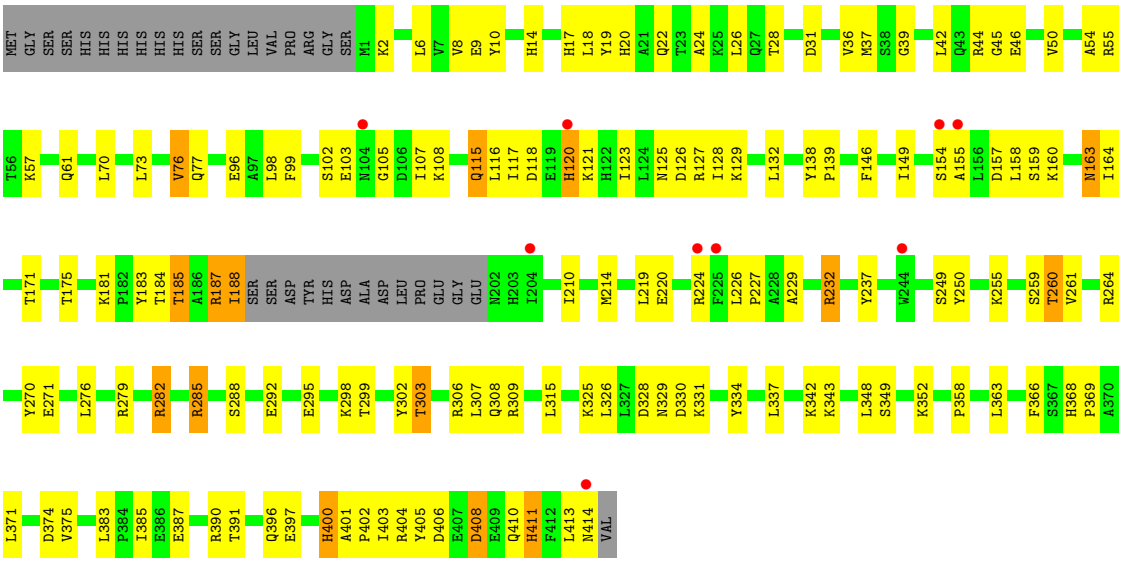
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	39	39	39	0	0
			Total	O		
3	B	28	28	28	0	0

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.

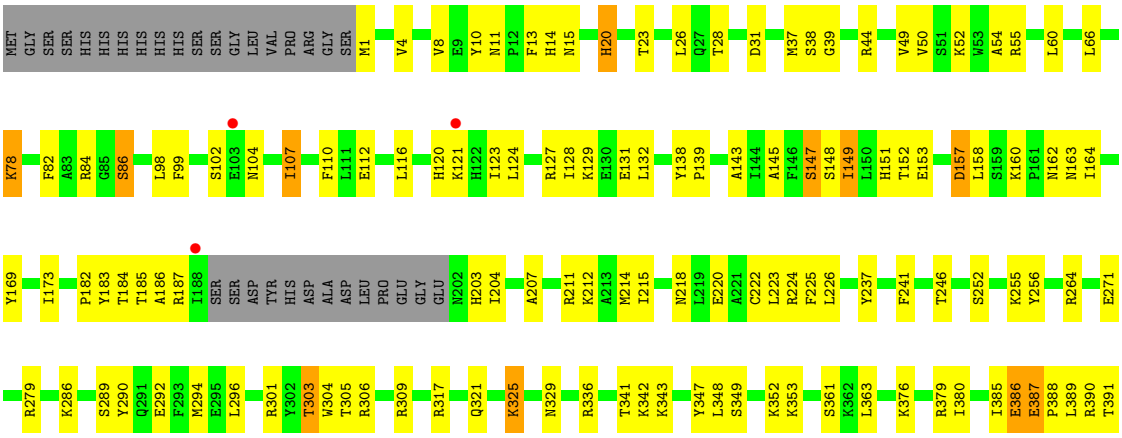
• Molecule 1: UPF0348 protein B4417_3650

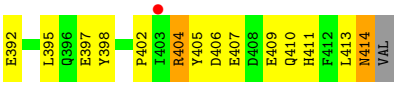
Chain A:



• Molecule 1: UPF0348 protein B4417_3650

Chain B:




E392
L395
Q396
E397
Y398
P402
I403
R404
Y405
D406
E407
D408
E409
Q410
H411
F412
L413
N414
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.00Å 68.01Å 211.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.10 48.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.97-2.10) 99.9 (48.97-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.202 , 0.243 0.205 , 0.249	Depositor DCC
R_{free} test set	2918 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.478 for k,h,-l	Xtriage
Reported twinning fraction	0.500 for -k,-h,-l	Depositor
Outliers	0 of 58350 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: APC

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	0.36	0/3274	0.55	0/4423
1	B	0.36	0/3274	0.56	0/4423
All	All	0.36	0/6548	0.56	0/8846

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	ASP	Peptide
1	B	409	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	3205	0	3232	117	1
1	B	3205	0	3232	99	1
2	A	31	0	14	11	0
2	B	31	0	14	3	0
3	A	39	0	0	6	0
3	B	28	0	0	2	0
All	All	6539	0	6492	210	1

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 16.

All (210) 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:19:TYR:CG	1:A:188:ILE:HD11	1.98	0.98
1:A:404:ARG:HE	1:A:413:LEU:HD12	1.40	0.85
1:A:229:ALA:HA	1:A:232:ARG:HD2	1.59	0.82
1:B:211:ARG:HA	1:B:214:MET:HE2	1.61	0.81
1:B:301:ARG:O	1:B:306:ARG:NH1	2.17	0.77
1:A:107:ILE:HD13	1:A:183:TYR:HA	1.66	0.76
1:B:49:VAL:HG12	1:B:50:VAL:HG23	1.66	0.76
1:A:102:SER:O	1:A:187:ARG:HG2	1.86	0.76
1:B:157:ASP:HB2	1:B:160:LYS:HG2	1.70	0.74
1:B:303:THR:HG23	1:B:306:ARG:H	1.54	0.73
1:A:188:ILE:HG13	2:A:1001:APC:HN62	1.54	0.72
1:B:44:ARG:NH2	2:B:1001:APC:O1B	2.22	0.71
1:B:143:ALA:O	1:B:147:SER:OG	2.08	0.71
1:A:121:LYS:NZ	3:A:1104:HOH:O	2.21	0.71
1:B:379:ARG:NH2	1:B:398:TYR:OH	2.23	0.71
1:B:220:GLU:HA	1:B:223:LEU:HD23	1.73	0.70
1:A:214:MET:HG2	1:A:219:LEU:HD13	1.73	0.70
1:B:212:LYS:HA	1:B:215:ILE:HD12	1.74	0.69
1:B:11:ASN:O	1:B:211:ARG:NH1	2.26	0.68
1:A:255:LYS:NZ	1:B:387:GLU:OE1	2.27	0.68
1:A:39:GLY:O	1:A:55:ARG:NH2	2.25	0.68
1:B:151:HIS:O	1:B:151:HIS:ND1	2.28	0.67
1:A:285:ARG:O	3:A:1102:HOH:O	2.13	0.66
1:A:400:HIS:O	3:A:1101:HOH:O	2.13	0.66
1:A:342:LYS:NZ	1:A:408:ASP:OD2	2.28	0.65
1:A:73:LEU:O	1:A:77:GLN:NE2	2.26	0.65
1:A:57:LYS:HG2	1:A:403:ILE:HG21	1.79	0.65
1:B:102:SER:HA	1:B:162:ASN:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ARG:NH1	1:B:361:SER:O	2.30	0.64
1:B:60:LEU:O	3:B:1101:HOH:O	2.15	0.64
1:B:38:SER:O	1:B:55:ARG:NH2	2.32	0.63
1:B:124:LEU:HD21	1:B:149:ILE:HD11	1.81	0.63
1:B:52:LYS:NZ	1:B:397:GLU:OE2	2.25	0.62
1:A:405:TYR:CE1	1:A:410:GLN:HA	2.34	0.62
1:A:125:ASN:HA	1:A:128:ILE:HD12	1.82	0.61
1:A:391:THR:OG1	1:B:255:LYS:NZ	2.34	0.61
1:A:8:VAL:HG12	2:A:1001:APC:H5'1	1.82	0.61
1:B:129:LYS:HA	1:B:132:LEU:HB2	1.83	0.61
1:A:187:ARG:HA	2:A:1001:APC:C2	2.31	0.60
1:A:406:ASP:HB3	1:A:411:HIS:HB2	1.83	0.60
1:A:107:ILE:HG12	1:A:184:THR:HG22	1.83	0.60
1:A:285:ARG:NH2	3:A:1106:HOH:O	2.24	0.60
1:A:45:GLY:O	1:A:308:GLN:HG2	2.02	0.60
1:A:220:GLU:N	1:A:220:GLU:OE1	2.34	0.59
1:B:107:ILE:HG23	1:B:184:THR:HG22	1.85	0.59
1:B:321:GLN:O	1:B:325:LYS:HB3	2.03	0.58
1:B:387:GLU:OE1	1:B:391:THR:OG1	2.22	0.56
1:A:154:SER:N	1:A:155:ALA:HA	2.19	0.56
1:B:211:ARG:O	1:B:215:ILE:HG13	2.05	0.56
1:B:157:ASP:OD2	1:B:157:ASP:N	2.31	0.56
1:B:405:TYR:CE1	1:B:410:GLN:HA	2.41	0.56
1:A:103:GLU:OE1	1:A:163:ASN:ND2	2.27	0.55
1:A:405:TYR:HE1	1:A:410:GLN:HA	1.71	0.55
1:A:19:TYR:CG	1:A:188:ILE:CD1	2.84	0.55
1:A:188:ILE:O	2:A:1001:APC:N6	2.39	0.55
1:B:98:LEU:O	1:B:183:TYR:N	2.35	0.55
1:B:50:VAL:HG22	1:B:237:TYR:CD2	2.41	0.55
1:B:387:GLU:OE2	1:B:390:ARG:NH1	2.40	0.55
1:A:19:TYR:CD1	1:A:188:ILE:HD11	2.41	0.55
1:A:326:LEU:HD21	1:A:369:PRO:HB2	1.87	0.54
1:B:405:TYR:HE1	1:B:410:GLN:HA	1.72	0.54
1:B:406:ASP:N	1:B:411:HIS:O	2.37	0.54
1:A:126:ASP:O	1:A:129:LYS:HB3	2.08	0.53
1:B:138:TYR:HB3	1:B:139:PRO:HD3	1.89	0.53
1:A:188:ILE:CG1	2:A:1001:APC:HN62	2.19	0.53
1:B:31:ASP:O	1:B:343:LYS:NZ	2.27	0.53
1:A:17:HIS:HE2	2:A:1001:APC:H3A1	1.74	0.53
1:A:76:VAL:HG12	1:A:309:ARG:HG2	1.90	0.53
1:A:329:ASN:ND2	1:A:331:LYS:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:O	1:A:175:THR:HG23	2.08	0.53
1:A:337:LEU:HG	1:A:402:PRO:HB3	1.90	0.53
1:B:279:ARG:NE	1:B:296:LEU:O	2.32	0.53
1:A:385:ILE:HB	1:A:390:ARG:HB2	1.91	0.52
1:B:120:HIS:O	1:B:123:ILE:N	2.42	0.52
1:A:57:LYS:O	1:A:61:GLN:NE2	2.42	0.52
1:A:10:TYR:O	1:A:55:ARG:HD2	2.10	0.52
1:B:152:THR:OG1	1:B:153:GLU:N	2.43	0.52
1:A:17:HIS:HE2	2:A:1001:APC:C3A	2.22	0.52
1:A:132:LEU:HD21	1:A:138:TYR:HA	1.91	0.52
1:B:145:ALA:O	1:B:148:SER:OG	2.19	0.52
1:A:401:ALA:HB1	1:A:402:PRO:HD2	1.92	0.51
1:A:390:ARG:NH2	1:B:252:SER:OG	2.30	0.51
1:A:219:LEU:N	1:A:220:GLU:OE1	2.43	0.51
1:A:8:VAL:O	1:A:37:MET:HA	2.11	0.51
2:A:1001:APC:H3A2	3:A:1125:HOH:O	2.09	0.51
1:B:116:LEU:O	1:B:120:HIS:ND1	2.42	0.51
1:A:102:SER:C	1:A:187:ARG:HG2	2.30	0.51
1:B:14:HIS:HA	1:B:226:LEU:HD23	1.92	0.50
1:A:103:GLU:CD	1:A:163:ASN:HD21	2.12	0.50
1:B:127:ARG:O	1:B:131:GLU:HG2	2.10	0.50
1:A:334:TYR:OH	1:A:374:ASP:OD2	2.18	0.50
1:A:36:VAL:HG22	1:A:70:LEU:HB2	1.94	0.50
1:A:115:GLN:HA	1:A:118:ASP:HB3	1.92	0.50
1:A:383:LEU:HA	1:A:390:ARG:HE	1.77	0.50
1:A:285:ARG:CZ	1:B:379:ARG:HG2	2.42	0.49
1:B:303:THR:OG1	1:B:304:TRP:N	2.44	0.49
1:B:112:GLU:O	1:B:116:LEU:N	2.44	0.49
1:B:10:TYR:CD2	1:B:13:PHE:HD1	2.31	0.49
1:A:19:TYR:CD2	1:A:188:ILE:HD11	2.47	0.49
1:B:84:ARG:NH2	1:B:329:ASN:O	2.46	0.49
1:B:290:TYR:O	1:B:294:MET:HG2	2.13	0.49
1:A:28:THR:HA	1:A:183:TYR:CE1	2.48	0.48
1:A:28:THR:HG22	1:A:183:TYR:CG	2.48	0.48
1:A:105:GLY:HA2	1:A:185:THR:HA	1.95	0.48
1:B:50:VAL:CG1	1:B:54:ALA:HB3	2.44	0.48
1:A:116:LEU:O	1:A:120:HIS:HB2	2.13	0.48
1:B:187:ARG:HA	2:B:1001:APC:N1	2.29	0.48
1:A:330:ASP:OD1	1:A:331:LYS:N	2.46	0.48
1:B:50:VAL:HG13	1:B:237:TYR:CD1	2.47	0.48
1:B:397:GLU:OE1	3:B:1103:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:OG	1:A:160:LYS:N	2.47	0.47
1:B:8:VAL:O	1:B:37:MET:HA	2.14	0.47
1:A:9:GLU:HB3	1:A:42:LEU:HD13	1.96	0.47
1:A:187:ARG:HH21	2:A:1001:APC:H2'	1.78	0.47
1:B:14:HIS:CD2	1:B:207:ALA:HB2	2.48	0.47
1:A:50:VAL:HG22	1:A:237:TYR:CG	2.48	0.47
1:B:78:LYS:H	1:B:78:LYS:HG2	1.33	0.47
1:B:120:HIS:HA	1:B:123:ILE:HD13	1.96	0.47
1:B:98:LEU:HD23	1:B:173:ILE:HD11	1.95	0.47
1:A:375:VAL:HG13	1:A:397:GLU:HG2	1.97	0.47
1:B:241:PHE:HA	1:B:389:LEU:HD13	1.97	0.47
1:A:127:ARG:HA	1:A:127:ARG:HD2	1.77	0.47
1:A:187:ARG:HA	2:A:1001:APC:N1	2.28	0.47
1:A:250:TYR:HB3	1:A:315:LEU:HD11	1.96	0.46
1:A:349:SER:OG	3:A:1103:HOH:O	2.21	0.46
1:B:10:TYR:OH	1:B:20:HIS:HE1	1.98	0.46
1:A:303:THR:HG23	1:A:306:ARG:HB2	1.97	0.46
1:A:73:LEU:HD22	1:A:326:LEU:HB3	1.97	0.46
1:A:279:ARG:HG3	1:A:282:ARG:NH1	2.30	0.46
1:B:39:GLY:O	1:B:52:LYS:HB3	2.16	0.46
1:B:341:THR:HB	1:B:407:GLU:HG2	1.97	0.46
1:B:10:TYR:O	1:B:55:ARG:HD2	2.14	0.46
1:A:121:LYS:HD3	1:A:121:LYS:HA	1.67	0.46
1:A:276:LEU:HD22	1:A:302:TYR:CE1	2.50	0.46
1:A:50:VAL:HG13	1:A:54:ALA:HB3	1.97	0.46
1:A:224:ARG:NH1	1:A:224:ARG:HB3	2.32	0.45
1:A:24:ALA:HA	1:A:99:PHE:CE1	2.51	0.45
1:B:82:PHE:O	1:B:86:SER:OG	2.25	0.45
1:A:19:TYR:CB	1:A:188:ILE:HD11	2.44	0.45
1:A:18:LEU:O	1:A:22:GLN:HG3	2.17	0.45
1:B:102:SER:OG	1:B:184:THR:OG1	2.33	0.45
1:A:158:LEU:HB3	1:A:164:ILE:HD11	1.99	0.45
1:B:1:MET:HG2	1:B:347:TYR:HD1	1.82	0.45
1:A:363:LEU:HD11	1:A:397:GLU:HG3	1.99	0.45
1:A:50:VAL:HG22	1:A:237:TYR:CD2	2.52	0.44
1:B:404:ARG:HG2	1:B:414:ASN:HD21	1.81	0.44
1:A:154:SER:H	1:A:155:ALA:HA	1.81	0.44
1:A:366:PHE:CE2	1:A:368:HIS:HB2	2.53	0.44
1:A:371:LEU:HD12	1:A:374:ASP:HB2	1.98	0.44
1:B:15:ASN:HB3	1:B:204:ILE:HG12	1.99	0.44
1:B:50:VAL:HG22	1:B:237:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:TYR:O	1:B:173:ILE:HG13	2.17	0.44
1:B:128:ILE:HG13	1:B:145:ALA:CB	2.48	0.43
1:B:214:MET:HA	1:B:218:ASN:O	2.18	0.43
1:B:392:GLU:O	1:B:395:LEU:HB2	2.18	0.43
1:B:342:LYS:HB2	1:B:407:GLU:HG3	2.00	0.43
1:A:371:LEU:O	1:A:375:VAL:HG23	2.19	0.43
1:B:376:LYS:O	1:B:380:ILE:HG12	2.19	0.43
1:B:385:ILE:HG22	1:B:386:GLU:O	2.18	0.43
1:A:6:LEU:HD22	1:A:20:HIS:CD2	2.54	0.43
1:A:187:ARG:NH2	2:A:1001:APC:O1B	2.42	0.43
1:B:102:SER:O	1:B:186:ALA:HA	2.19	0.43
1:A:298:LYS:HA	1:A:307:LEU:HD11	2.00	0.43
1:B:78:LYS:HE3	1:B:271:GLU:OE2	2.18	0.43
1:B:222:CYS:O	1:B:225:PHE:N	2.51	0.43
1:B:107:ILE:O	1:B:110:PHE:HB2	2.19	0.43
1:B:158:LEU:HD23	1:B:163:ASN:HB3	2.00	0.43
1:A:6:LEU:HD22	1:A:20:HIS:NE2	2.33	0.42
1:A:138:TYR:HB3	1:A:139:PRO:HD3	2.01	0.42
1:A:387:GLU:OE1	1:A:390:ARG:HD2	2.19	0.42
1:A:404:ARG:NE	1:A:413:LEU:HD12	2.22	0.42
1:A:210:ILE:HG21	1:A:226:LEU:HD11	2.02	0.42
1:A:288:SER:CB	1:B:387:GLU:HG2	2.50	0.42
1:A:348:LEU:O	1:A:352:LYS:N	2.53	0.42
1:B:98:LEU:HB3	1:B:182:PRO:HA	2.01	0.42
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.78	0.42
1:B:151:HIS:O	1:B:151:HIS:CG	2.72	0.42
1:A:232:ARG:H	1:A:232:ARG:HG3	1.68	0.42
1:B:363:LEU:HD23	1:B:363:LEU:HA	1.79	0.42
1:A:163:ASN:OD1	1:A:163:ASN:N	2.53	0.42
1:A:44:ARG:O	1:A:308:GLN:HB3	2.20	0.41
1:B:15:ASN:ND2	1:B:224:ARG:O	2.53	0.41
1:B:158:LEU:O	1:B:164:ILE:HD11	2.19	0.41
1:A:358:PRO:HG2	1:A:366:PHE:CE1	2.56	0.41
1:A:383:LEU:HD11	1:B:256:TYR:CD1	2.56	0.41
1:B:4:VAL:HG21	1:B:28:THR:HG21	2.02	0.41
1:A:302:TYR:CD2	1:A:306:ARG:HD3	2.55	0.41
1:A:2:LYS:HD3	1:A:96:GLU:OE2	2.20	0.41
1:B:23:THR:HA	1:B:26:LEU:HB2	2.03	0.41
2:B:1001:APC:H2'	2:B:1001:APC:O2B	2.21	0.41
1:A:157:ASP:OD2	1:A:160:LYS:NZ	2.46	0.41
1:A:383:LEU:HD11	1:B:256:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PHE:HD1	1:B:183:TYR:HB2	1.84	0.41
1:A:292:GLU:O	1:A:295:GLU:HB2	2.21	0.41
1:A:123:ILE:H	1:A:123:ILE:HG12	1.62	0.41
1:A:270:TYR:O	1:A:271:GLU:HB2	2.21	0.41
1:B:121:LYS:HD3	1:B:124:LEU:HD12	2.01	0.41
1:B:286:LYS:H	1:B:286:LYS:HG2	1.62	0.41
1:B:292:GLU:O	1:B:296:LEU:HG	2.20	0.41
1:B:305:THR:O	1:B:309:ARG:HG3	2.21	0.41
1:A:14:HIS:HA	1:A:227:PRO:HD2	2.03	0.40
1:A:385:ILE:O	1:A:390:ARG:HB2	2.21	0.40
1:B:361:SER:HB3	1:B:402:PRO:HG3	2.03	0.40
1:A:260:THR:HB	1:B:317:ARG:HG3	2.03	0.40
1:B:388:PRO:O	1:B:392:GLU:HG3	2.22	0.40
1:A:396:GLN:O	1:A:400:HIS:N	2.28	0.40
1:A:406:ASP:HB3	1:A:411:HIS:CB	2.50	0.40
1:B:349:SER:HA	1:B:352:LYS:HD2	2.03	0.40
1:A:98:LEU:HD12	1:A:99:PHE:N	2.36	0.40
1:A:117:ILE:HG22	1:A:121:LYS:HE2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:NH1	1:B:153:GLU:OE1[4_545]	2.19	0.01

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	397/434 (92%)	380 (96%)	17 (4%)	0	100	100
1	B	397/434 (92%)	375 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	794/868 (92%)	755 (95%)	39 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	345/373 (92%)	316 (92%)	29 (8%)	11 7
1	B	345/373 (92%)	322 (93%)	23 (7%)	16 13
All	All	690/746 (92%)	638 (92%)	52 (8%)	13 10

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	31	ASP
1	A	46	GLU
1	A	76	VAL
1	A	108	LYS
1	A	115	GLN
1	A	120	HIS
1	A	146	PHE
1	A	149	ILE
1	A	163	ASN
1	A	181	LYS
1	A	185	THR
1	A	187	ARG
1	A	188	ILE
1	A	232	ARG
1	A	249	SER
1	A	259	SER
1	A	260	THR
1	A	261	VAL
1	A	282	ARG

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Mol	Chain	Res	Type
1	A	285	ARG
1	A	299	THR
1	A	303	THR
1	A	325	LYS
1	A	328	ASP
1	A	343	LYS
1	A	400	HIS
1	A	411	HIS
1	A	414	ASN
1	B	20	HIS
1	B	66	LEU
1	B	78	LYS
1	B	86	SER
1	B	104	ASN
1	B	107	ILE
1	B	147	SER
1	B	149	ILE
1	B	157	ASP
1	B	185	THR
1	B	203	HIS
1	B	246	THR
1	B	264	ARG
1	B	289	SER
1	B	303	THR
1	B	325	LYS
1	B	348	LEU
1	B	353	LYS
1	B	386	GLU
1	B	387	GLU
1	B	404	ARG
1	B	413	LEU
1	B	414	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	HIS
1	B	104	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 monosaccharides 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	APC	B	1001	-	27,33,33	1.27	5 (18%)	31,52,52	1.62	6 (19%)
2	APC	A	1001	-	27,33,33	1.25	3 (11%)	31,52,52	1.63	6 (19%)

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	APC	B	1001	-	-	1/15/38/38	0/3/3/3
2	APC	A	1001	-	-	2/15/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	APC	PB-O3B	2.92	1.61	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	APC	PA-O5'	2.87	1.61	1.57
2	A	1001	APC	PA-O5'	2.59	1.61	1.57
2	B	1001	APC	C5-C4	2.44	1.47	1.40
2	A	1001	APC	C5-C4	2.41	1.47	1.40
2	B	1001	APC	PB-O2B	-2.33	1.50	1.56
2	B	1001	APC	PA-O2A	-2.19	1.51	1.56
2	B	1001	APC	PB-O3B	2.15	1.60	1.58

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	APC	O2A-PA-O1A	4.30	124.41	110.07
2	B	1001	APC	PB-O3B-PG	-3.89	118.93	132.62
2	B	1001	APC	O2A-PA-O1A	3.65	122.25	110.07
2	B	1001	APC	N3-C2-N1	-3.40	123.36	128.68
2	A	1001	APC	C4-C5-N7	-3.28	105.98	109.40
2	A	1001	APC	PB-O3B-PG	-3.27	121.10	132.62
2	B	1001	APC	C4-C5-N7	-2.97	106.30	109.40
2	A	1001	APC	N3-C2-N1	-2.93	124.10	128.68
2	A	1001	APC	O2B-PB-O1B	2.78	119.35	110.07
2	B	1001	APC	O2B-PB-O1B	2.59	118.71	110.07
2	B	1001	APC	C2-N1-C6	2.06	122.27	118.75
2	A	1001	APC	C1'-N9-C4	-2.00	123.12	126.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	APC	PA-C3A-PB-O1B
2	A	1001	APC	PA-C3A-PB-O3B
2	B	1001	APC	C5'-O5'-PA-O1A

There are no ring outliers.

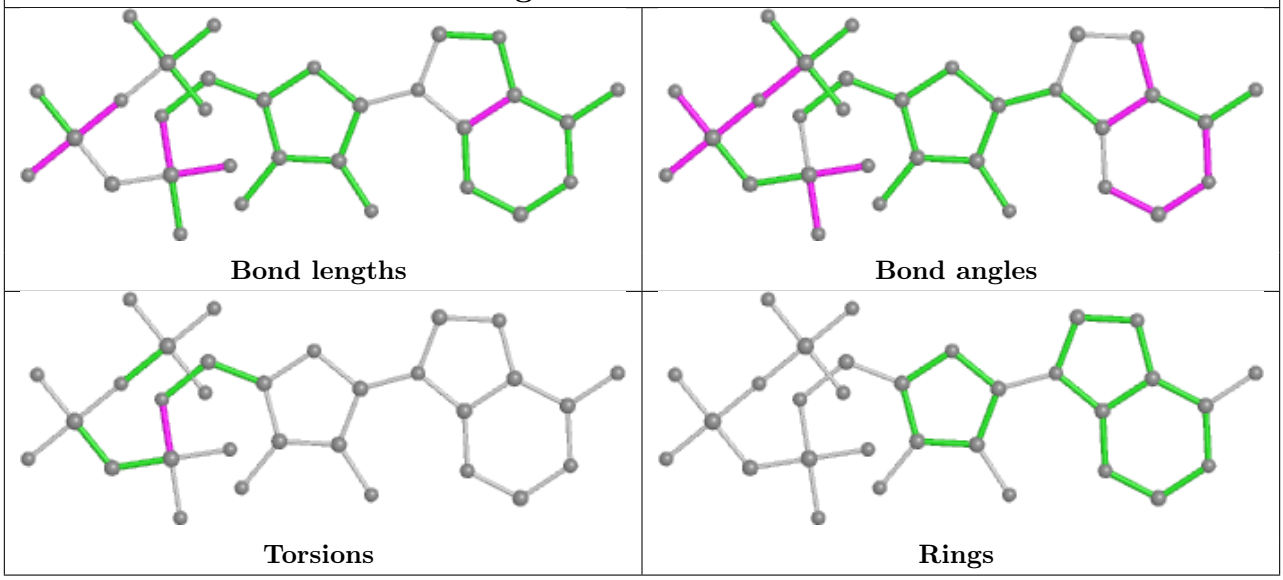
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	APC	3	0
2	A	1001	APC	11	0

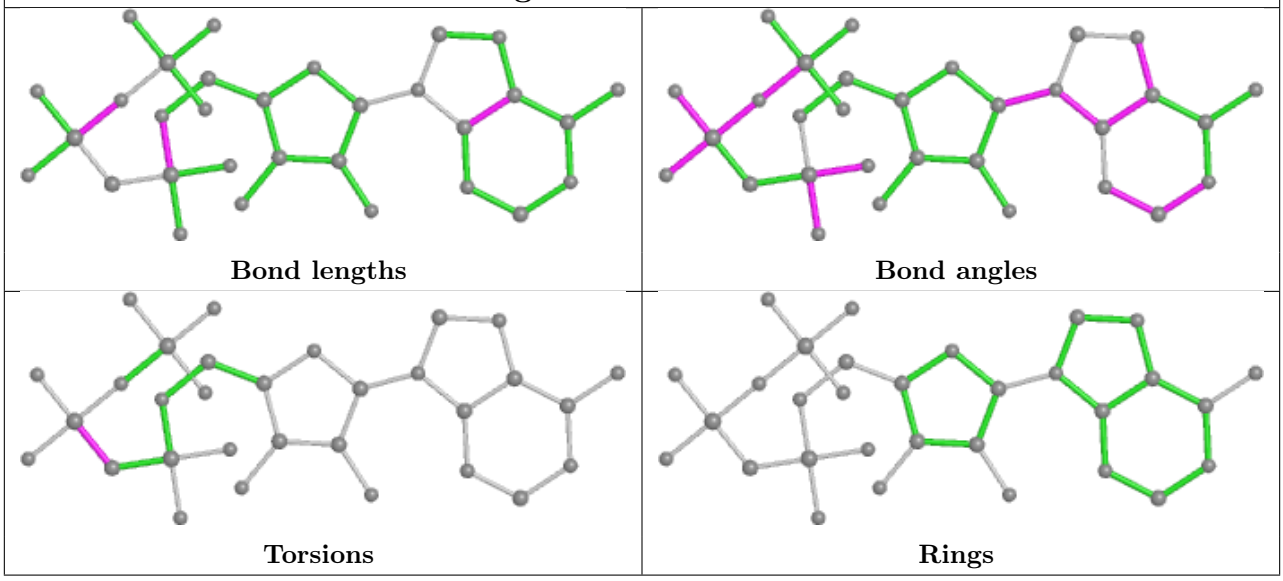
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 APC B 1001



Ligand APC A 1001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	401/434 (92%)	-0.05	9 (2%)	62	66	34, 60, 100, 142	0
1	B	401/434 (92%)	-0.13	4 (0%)	82	85	35, 59, 92, 123	0
All	All	802/868 (92%)	-0.09	13 (1%)	72	75	34, 60, 95, 142	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ALA	8.4
1	B	188	ILE	5.1
1	A	224	ARG	3.5
1	A	204	ILE	3.1
1	A	154	SER	3.1
1	A	244	TRP	2.9
1	B	403	ILE	2.9
1	A	225	PHE	2.5
1	A	120	HIS	2.3
1	A	104	ASN	2.3
1	B	103	GLU	2.3
1	A	414	ASN	2.2
1	B	121	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

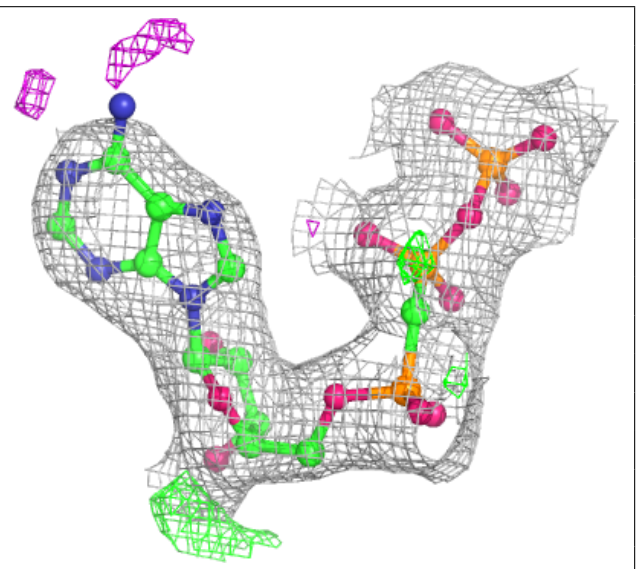
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

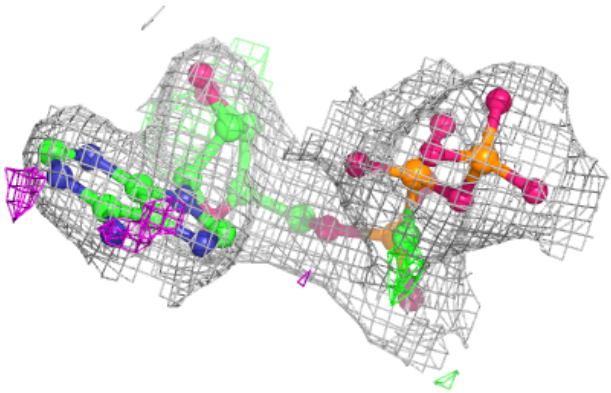
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	APC	A	1001	31/31	0.94	0.11	52,64,71,78	0
2	APC	B	1001	31/31	0.95	0.11	48,60,176,176	0

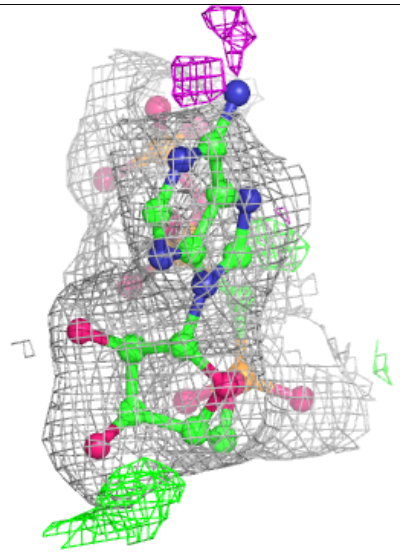
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC A 1001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

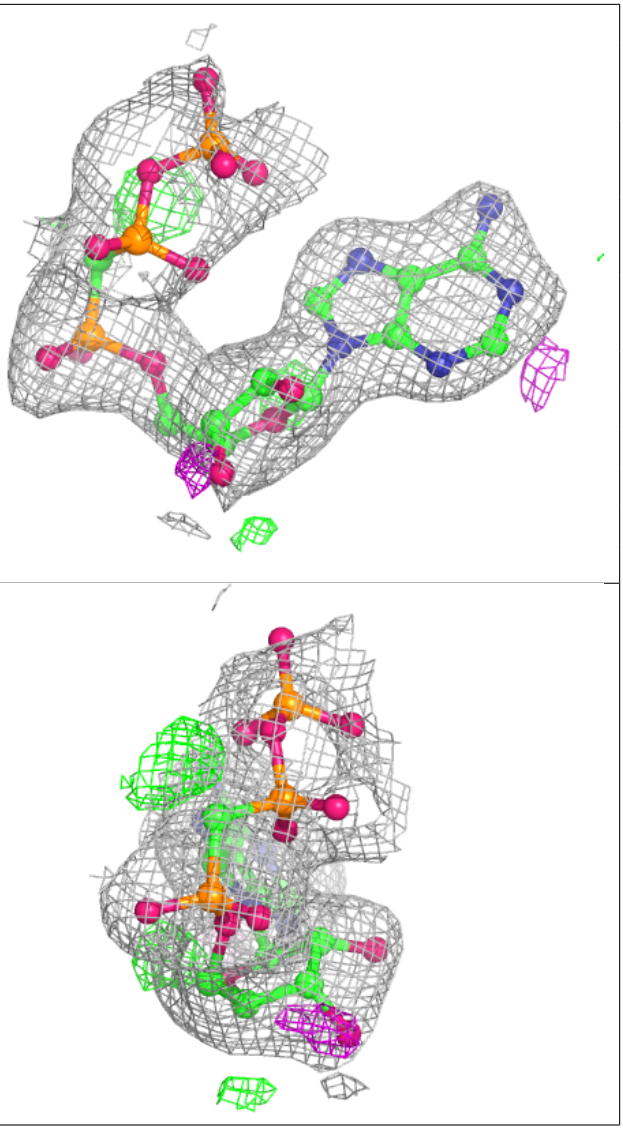






Electron density around APC B 1001:

$2mF_o$-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.