Full wwPDB X-ray Structure Validation Report (i)

Jun 14, 2020 – 10:11 pm BST

PDB ID	:	3DDQ
Title	:	Structure of phosphorylated Thr160 CDK2/cyclin A in complex with the inhibitor roscovitine
Authors	:	Echalier, A.; Endicott, J.A.
Deposited on	:	2008-06-06
Resolution	:	1.80 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 (i)) were used in the production of this report:

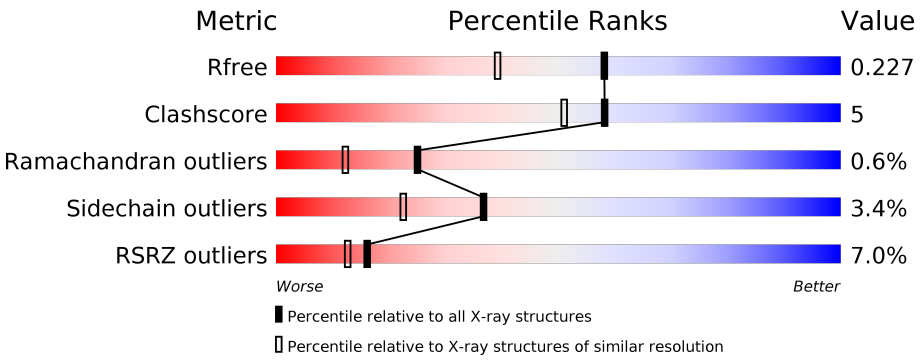
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	299	7%, 88%, 10%
1	C	299	7%, 75%, 12%, 11%
2	B	269	4%, 90%, 7%
2	D	269	9%, 91%, 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SGM	B	440	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9800 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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	297	2405	1562	410	424	1	8	0	2	0
1	C	267	2179	1411	377	383	1	7	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	262	2135	1385	347	393	10	0	4	0
2	D	269	2188	1414	366	398	10	0	1	0

There are 14 discrepancies between the modelled and reference sequences:

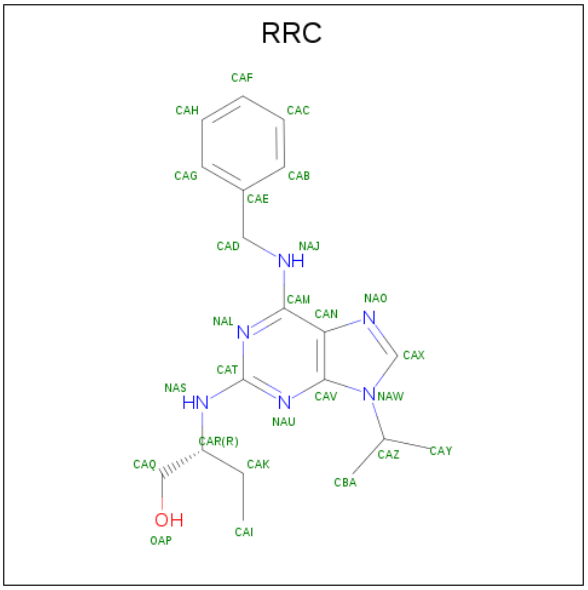
Chain	Residue	Modelled	Actual	Comment	Reference
B	433	HIS	-	EXPRESSION TAG	UNP P30274
B	434	HIS	-	EXPRESSION TAG	UNP P30274
B	435	HIS	-	EXPRESSION TAG	UNP P30274
B	436	HIS	-	EXPRESSION TAG	UNP P30274
B	437	HIS	-	EXPRESSION TAG	UNP P30274
B	438	HIS	-	EXPRESSION TAG	UNP P30274
B	439	HIS	-	EXPRESSION TAG	UNP P30274
D	433	HIS	-	EXPRESSION TAG	UNP P30274
D	434	HIS	-	EXPRESSION TAG	UNP P30274
D	435	HIS	-	EXPRESSION TAG	UNP P30274

Continued on next page...

Continued from previous page...

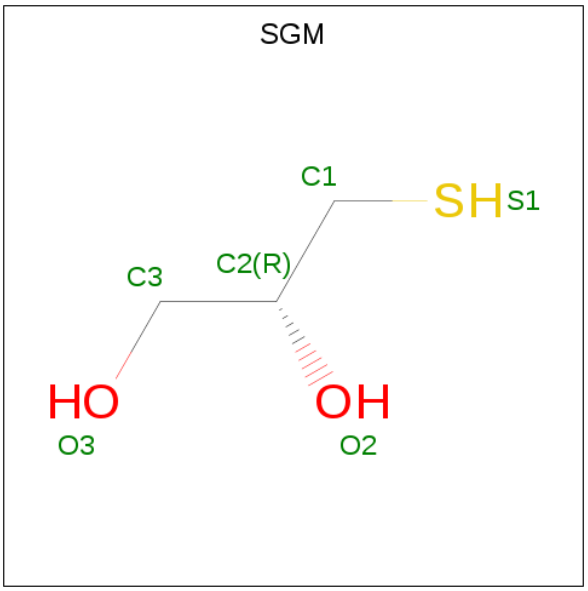
Chain	Residue	Modelled	Actual	Comment	Reference
D	436	HIS	-	EXPRESSION TAG	UNP P30274
D	437	HIS	-	EXPRESSION TAG	UNP P30274
D	438	HIS	-	EXPRESSION TAG	UNP P30274
D	439	HIS	-	EXPRESSION TAG	UNP P30274

- Molecule 3 is R-ROSCOVITINE (three-letter code: RRC) (formula: $C_{19}H_{26}N_6O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	26	19	6	1	0	0
			Total	C	N	O		
3	C	1	26	19	6	1	0	0

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	B	1	6	3	2	1	0	0
			Total	C	O	S		
4	B	1	6	3	2	1	0	0
			Total	C	O	S		
4	D	1	6	3	2	1	0	0

- Molecule 5 is water.

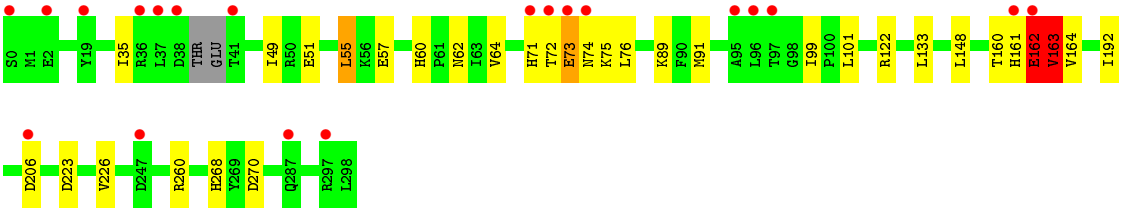
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	265	265	265	0	0
			Total	O		
5	B	219	219	219	0	0
			Total	O		
5	C	153	153	153	0	0
			Total	O		
5	D	186	186	186	0	0

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.

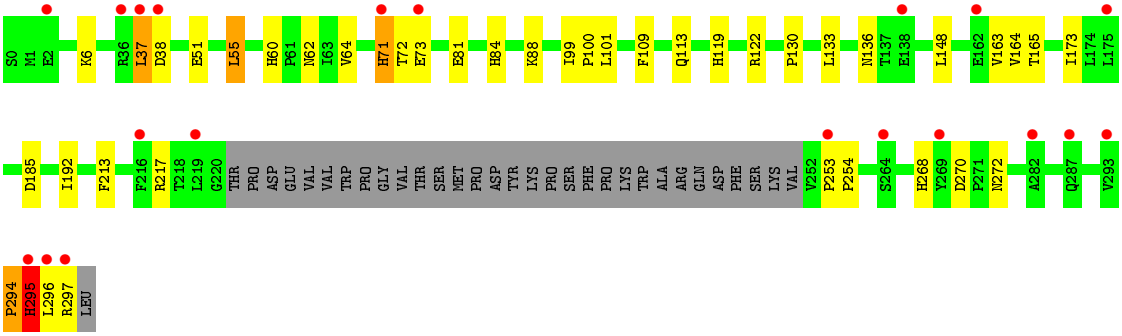
- Molecule 1: Cell division protein kinase 2

Chain A:



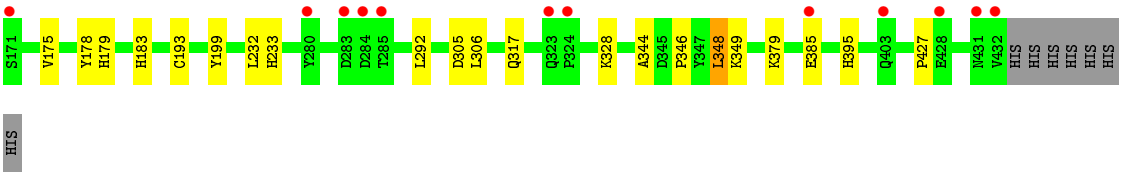
- Molecule 1: Cell division protein kinase 2

Chain C:



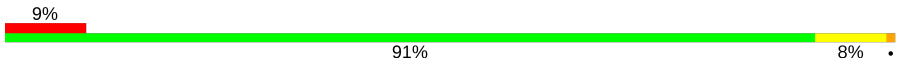
- Molecule 2: Cyclin-A2

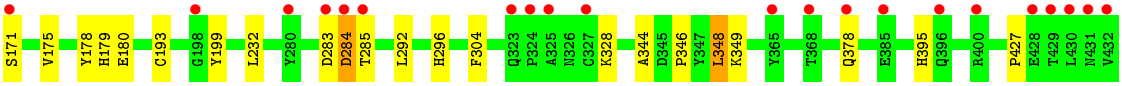
Chain B:

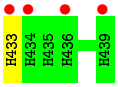


- Molecule 2: Cyclin-A2

Chain D:




S171
V175
Y178
H179
E180
C193
G198
Y199
L232
Y280
D283
D284
T285
L292
H296
F304
Q323
P324
A325
N326
C327
K328
A344
D345
P346
Y347
L348
K349
Y365
T368
Q378
E385
H395
Q396
R400
P427
E428
T429
L430
N431
V432


H433
H434
H435
H436
H439

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.42Å 133.38Å 147.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-1.80) 90.0 (19.90-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.229 0.194 , 0.227	Depositor DCC
R_{free} test set	4947 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9800	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: TPO, RRC, SGM

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	0.50	0/2460	0.62	4/3334 (0.1%)
1	C	0.40	0/2232	0.58	0/3019
2	B	0.40	0/2198	0.53	0/2989
2	D	0.38	0/2248	0.53	0/3056
All	All	0.42	0/9138	0.57	4/12398 (0.0%)

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
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162[A]	GLU	CA-C-N	-5.35	105.42	117.20
1	A	162[B]	GLU	CA-C-N	-5.35	105.42	117.20
1	A	162[A]	GLU	CA-C-O	5.21	131.03	120.10
1	A	162[B]	GLU	CA-C-O	5.21	131.03	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162[A]	GLU	Mainchain
1	A	162[B]	GLU	Mainchain
1	C	294	PRO	Peptide
1	C	37	LEU	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	2405	0	2459	27	0
1	C	2179	0	2245	37	0
2	B	2135	0	2165	12	0
2	D	2188	0	2192	16	0
3	A	26	0	25	2	0
3	C	26	0	25	3	0
4	B	12	0	16	2	0
4	D	6	0	8	1	0
5	A	265	0	0	3	0
5	B	219	0	0	3	0
5	C	153	0	0	4	0
5	D	186	0	0	3	0
All	All	9800	0	9135	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (87) 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)
2:B:193:CYS:SG	4:B:1:SGM:S1	2.51	1.02
1:C:37:LEU:HA	1:C:38:ASP:HB2	1.57	0.87
1:C:294:PRO:HA	1:C:295:HIS:HB3	1.60	0.82
1:A:73:GLU:HG3	1:A:74:ASN:H	1.45	0.80
1:A:73:GLU:CG	1:A:74:ASN:H	1.98	0.76
1:A:162[B]:GLU:HG3	1:A:163:VAL:H	1.50	0.75
1:A:60:HIS:HD2	1:A:62:ASN:H	1.33	0.75
1:A:60:HIS:CD2	1:A:62:ASN:H	2.07	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ASN:CG	2:D:171:SER:HB2	2.08	0.73
1:A:160:TPO:HG23	1:A:162[B]:GLU:HG2	1.71	0.72
1:C:295:HIS:CE1	1:C:296:LEU:HD13	2.26	0.70
1:C:60:HIS:HD2	1:C:62:ASN:H	1.38	0.69
1:A:161:HIS:HD2	5:A:411:HOH:O	1.75	0.69
1:A:64:VAL:HG21	3:A:299:RRC:HAY2	1.73	0.69
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.28	0.69
1:C:272:ASN:OD1	2:D:171:SER:HB2	1.92	0.69
1:C:60:HIS:CD2	1:C:62:ASN:H	2.13	0.66
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.59	0.66
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.76	0.66
1:C:268:HIS:HD2	1:C:270:ASP:H	1.44	0.65
3:A:299:RRC:HAR	5:A:504:HOH:O	1.99	0.61
1:C:71[A]:HIS:CD2	2:D:296:HIS:CE1	2.90	0.59
1:A:268:HIS:HD2	1:A:270:ASP:H	1.51	0.58
1:A:160:TPO:CG2	1:A:162[B]:GLU:HG2	2.33	0.58
2:D:175:VAL:CG1	2:D:178:TYR:HB2	2.33	0.58
2:D:193:CYS:SG	4:D:1:SGM:S1	2.36	0.57
2:D:395:HIS:HE1	2:D:427:PRO:O	1.88	0.57
1:C:295:HIS:ND1	1:C:296:LEU:HD13	2.19	0.57
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.87	0.57
1:A:162[B]:GLU:HG3	1:A:163:VAL:N	2.19	0.57
1:A:57:GLU:HG2	5:B:570:HOH:O	2.05	0.56
1:A:71:HIS:HD2	1:A:76:LEU:HD13	1.70	0.55
1:A:73:GLU:CG	1:A:74:ASN:N	2.68	0.54
1:C:173:ILE:HG23	5:C:361:HOH:O	2.08	0.54
1:C:99:ILE:HG23	1:C:295:HIS:HD2	1.73	0.53
2:D:346:PRO:O	2:D:349:LYS:HG2	2.09	0.52
1:C:72:THR:HG22	1:C:73[B]:GLU:H	1.73	0.52
2:B:305:ASP:HB3	4:B:1:SGM:H12	1.92	0.52
1:C:72:THR:HG22	1:C:73[A]:GLU:H	1.73	0.51
1:A:73:GLU:HG3	1:A:74:ASN:N	2.20	0.51
1:C:88:LYS:HB2	1:C:130:PRO:HB2	1.93	0.51
1:A:223:ASP:H	1:A:226:VAL:HG12	1.76	0.50
1:C:71[A]:HIS:CE1	2:D:304:PHE:HE2	2.30	0.50
1:C:100:PRO:HD2	1:C:295:HIS:CD2	2.46	0.50
1:C:295:HIS:O	1:C:296:LEU:HB2	2.12	0.49
1:C:71[A]:HIS:HD2	2:D:296:HIS:CE1	2.30	0.49
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.93	0.49
1:A:35:ILE:HB	1:A:76:LEU:HB3	1.95	0.49
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:VAL:HG12	2:D:178:TYR:HB2	1.94	0.48
1:C:64:VAL:HG21	3:C:299:RRC:HAY2	1.95	0.47
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.96	0.47
1:C:119:HIS:HD2	5:D:441:HOH:O	1.96	0.47
2:D:179:HIS:CE1	2:D:180:GLU:HG2	2.49	0.47
2:B:233:HIS:HD2	5:B:444:HOH:O	1.96	0.47
2:B:175[A]:VAL:HG12	2:B:178:TYR:HB2	1.96	0.47
2:B:183:HIS:HD2	5:B:637:HOH:O	1.97	0.47
1:C:294:PRO:HA	1:C:295:HIS:CB	2.39	0.46
2:B:346:PRO:O	2:B:349:LYS:HG2	2.16	0.45
2:B:179[B]:HIS:CE1	2:B:379:LYS:NZ	2.84	0.45
1:C:100:PRO:CD	1:C:295:HIS:CD2	3.00	0.45
1:A:260:ARG:HD3	5:A:369:HOH:O	2.15	0.45
1:A:223:ASP:H	1:A:226:VAL:CG1	2.29	0.45
2:D:284:ASP:N	5:D:531:HOH:O	2.49	0.45
2:D:285:THR:N	5:D:536:HOH:O	2.50	0.44
2:B:395:HIS:HE1	2:B:427:PRO:O	2.00	0.44
1:C:165:THR:HG22	5:C:331:HOH:O	2.17	0.44
1:C:253:PRO:HD2	1:C:254:PRO:HD3	1.99	0.44
1:C:99:ILE:HG23	1:C:295:HIS:CD2	2.51	0.43
3:C:299:RRC:HAG	5:C:323:HOH:O	2.18	0.43
1:C:99:ILE:HA	1:C:295:HIS:NE2	2.33	0.43
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.01	0.42
1:C:213:PHE:O	1:C:217:ARG:HG3	2.19	0.42
1:A:162[B]:GLU:CG	1:A:163:VAL:N	2.80	0.42
1:C:84:HIS:HD2	1:C:136:ASN:HA	1.84	0.42
2:D:175:VAL:HG11	2:D:178:TYR:HB2	2.00	0.42
1:C:51:GLU:HG3	1:C:55:LEU:HD22	2.00	0.42
1:C:71[A]:HIS:CE1	2:D:304:PHE:CE2	3.08	0.42
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.41
1:C:163:VAL:HG22	5:C:361:HOH:O	2.20	0.41
1:C:81:GLU:O	3:C:299:RRC:HAX	2.20	0.41
1:C:109:PHE:O	1:C:113:GLN:HG3	2.21	0.40
2:B:175[A]:VAL:CG1	2:B:178:TYR:HB2	2.50	0.40
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.02	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	294/299 (98%)	284 (97%)	5 (2%)	5 (2%)	9 2
1	C	267/299 (89%)	256 (96%)	9 (3%)	2 (1%)	22 10
2	B	264/269 (98%)	263 (100%)	1 (0%)	0	100 100
2	D	268/269 (100%)	266 (99%)	2 (1%)	0	100 100
All	All	1093/1136 (96%)	1069 (98%)	17 (2%)	7 (1%)	25 12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	162[A]	GLU
1	A	162[B]	GLU
1	A	163	VAL
1	A	164	VAL
1	C	164	VAL
1	C	295	HIS

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	263/263 (100%)	252 (96%)	11 (4%)	30 15
1	C	238/263 (90%)	229 (96%)	9 (4%)	33 18
2	B	239/242 (99%)	233 (98%)	6 (2%)	47 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	243/242 (100%)	234 (96%)	9 (4%)	34	19
All	All	983/1010 (97%)	948 (96%)	35 (4%)	37	20

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	72	THR
1	A	75	LYS
1	A	89	LYS
1	A	101	LEU
1	A	122	ARG
1	A	148	LEU
1	A	162[A]	GLU
1	A	162[B]	GLU
1	A	163	VAL
1	A	206	ASP
2	B	199	TYR
2	B	232	LEU
2	B	292	LEU
2	B	328	LYS
2	B	348	LEU
2	B	385	GLU
1	C	6	LYS
1	C	55	LEU
1	C	71[A]	HIS
1	C	71[B]	HIS
1	C	101	LEU
1	C	122	ARG
1	C	148	LEU
1	C	295	HIS
1	C	297	ARG
2	D	199	TYR
2	D	232	LEU
2	D	283	ASP
2	D	284	ASP
2	D	292	LEU
2	D	328	LYS
2	D	348	LEU
2	D	378	GLN
2	D	433	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	161	HIS
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	317	GLN
2	B	378	GLN
2	B	395	HIS
2	B	425	ASN
1	C	60	HIS
1	C	74	ASN
1	C	84	HIS
1	C	119	HIS
1	C	161	HIS
1	C	268	HIS
1	C	295	HIS
2	D	179	HIS
2	D	183	HIS
2	D	233	HIS
2	D	254	GLN
2	D	317	GLN
2	D	370	GLN
2	D	378	GLN
2	D	395	HIS
2	D	406	GLN
2	D	436	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	A	160	1	8,10,11	0.79	0	10,14,16	1.07	0
1	TPO	C	160	1	8,10,11	0.71	0	10,14,16	1.02	0

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
1	TPO	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	SGM	B	440	-	5,5,5	0.43	0	5,5,5	0.47	0
4	SGM	B	1	-	5,5,5	0.46	0	5,5,5	0.49	0
4	SGM	D	1	-	5,5,5	0.39	0	5,5,5	0.51	0
3	RRC	C	299	-	25,28,28	0.81	0	27,38,38	3.92	10 (37%)
3	RRC	A	299	-	25,28,28	0.86	1 (4%)	27,38,38	3.77	9 (33%)

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	SGM	B	440	-	-	0/4/4/4	-
4	SGM	B	1	-	-	2/4/4/4	-
4	SGM	D	1	-	-	0/4/4/4	-
3	RRC	C	299	-	-	0/17/17/17	0/3/3/3
3	RRC	A	299	-	-	1/17/17/17	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	299	RRC	CAM-NAL	2.35	1.36	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	299	RRC	CAZ-NAW-CAV	-12.30	112.55	127.15
3	C	299	RRC	CAX-NAW-CAZ	12.20	137.40	125.42
3	A	299	RRC	CAX-NAW-CAZ	11.79	137.00	125.42
3	A	299	RRC	CAZ-NAW-CAV	-11.56	113.42	127.15
3	C	299	RRC	CBA-CAZ-NAW	7.30	122.24	110.30
3	A	299	RRC	CBA-CAZ-NAW	6.28	120.57	110.30
3	A	299	RRC	NAU-CAT-NAL	-3.84	120.16	126.23
3	C	299	RRC	NAU-CAT-NAL	-3.52	120.66	126.23
3	A	299	RRC	CAT-NAU-CAV	3.17	118.88	115.28
3	C	299	RRC	CBA-CAZ-CAY	2.60	121.28	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	299	RRC	CAT-NAU-CAV	2.59	118.22	115.28
3	A	299	RRC	CAY-CAZ-NAW	2.43	114.27	110.30
3	A	299	RRC	CAT-NAL-CAM	2.39	121.87	116.39
3	A	299	RRC	CAV-CAN-NAO	-2.37	106.93	109.40
3	C	299	RRC	CAT-NAL-CAM	2.36	121.79	116.39
3	C	299	RRC	CAV-CAN-NAO	-2.33	106.97	109.40
3	A	299	RRC	CAD-NAJ-CAM	-2.16	120.22	123.11
3	C	299	RRC	CAN-CAM-NAL	-2.16	119.02	120.81
3	C	299	RRC	NAS-CAT-NAU	2.09	120.31	117.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	SGM	C1-C2-C3-O3
4	B	1	SGM	O2-C2-C3-O3
3	A	299	RRC	CAI-CAK-CAR-NAS

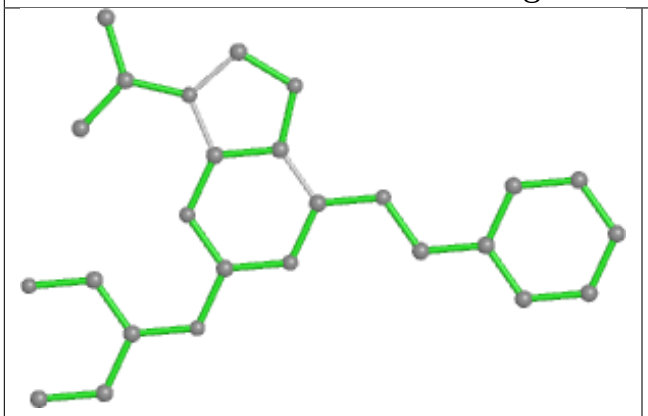
There are no ring outliers.

4 monomers are involved in 8 short contacts:

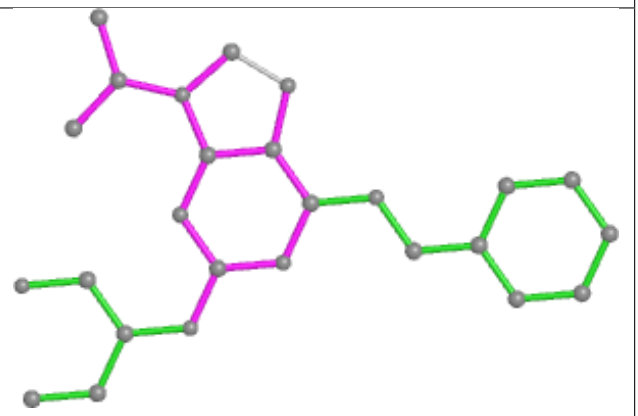
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	SGM	2	0
4	D	1	SGM	1	0
3	C	299	RRC	3	0
3	A	299	RRC	2	0

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 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.

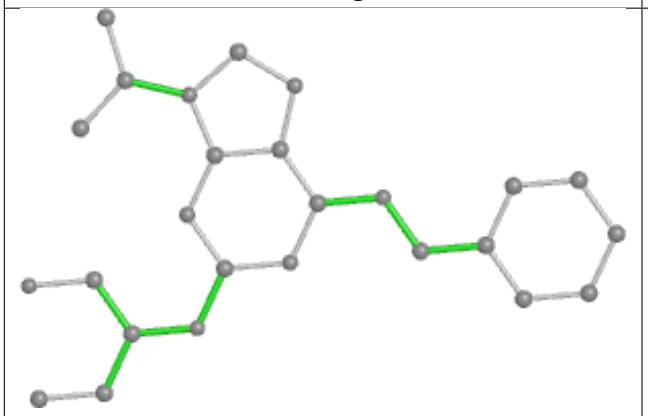
Ligand RRC C 299



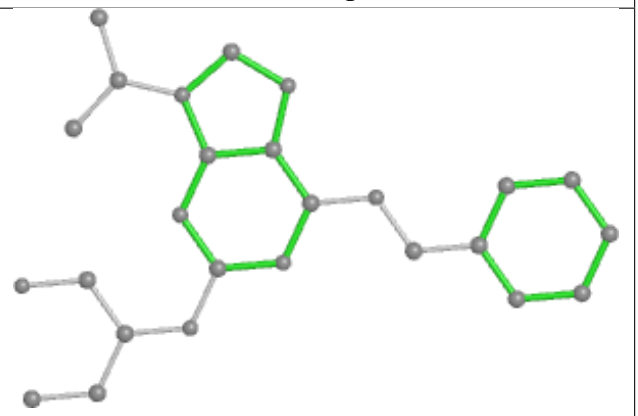
Bond lengths



Bond angles

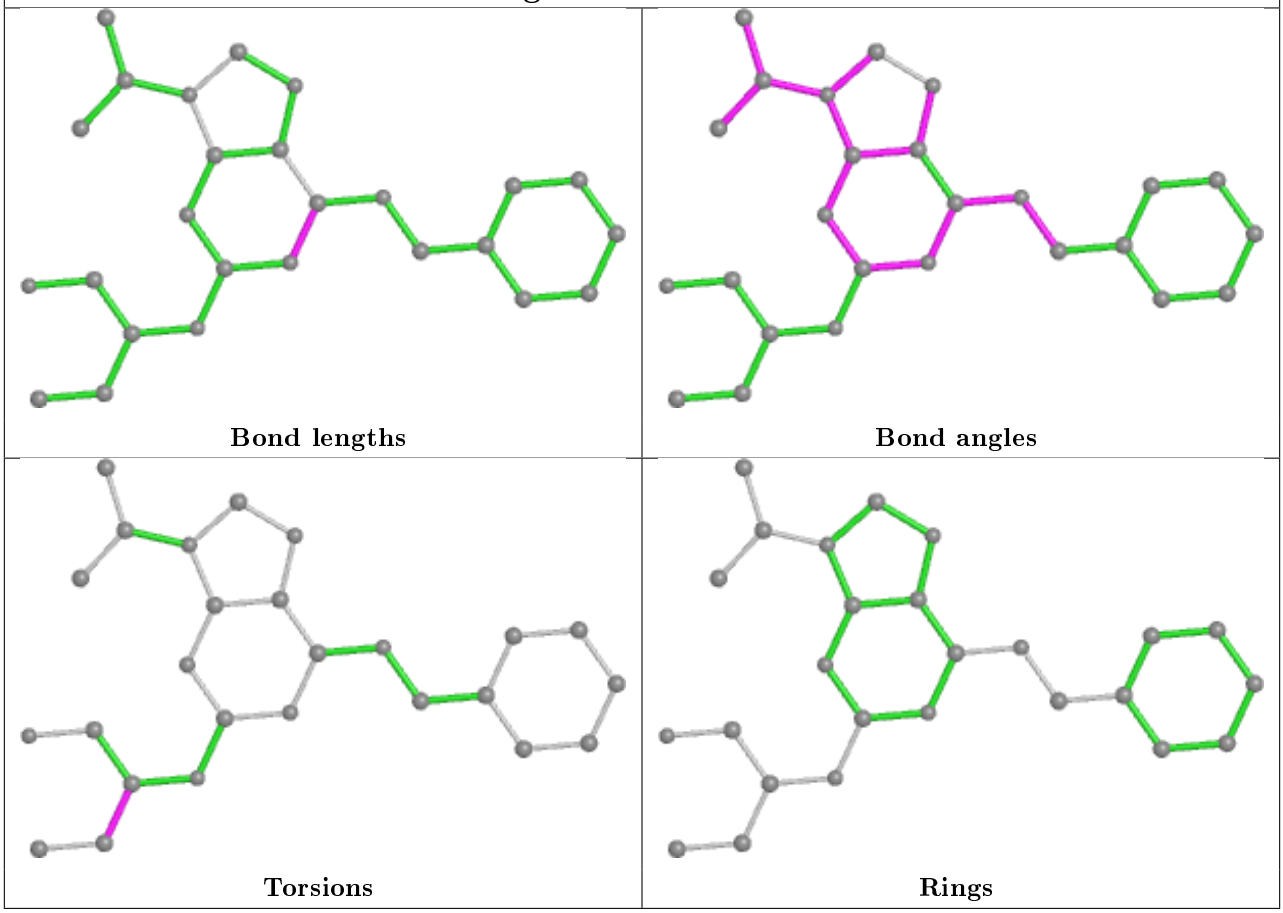


Torsions



Rings

Ligand RRC A 299



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	296/299 (98%)	0.12	20 (6%)	17	13	8, 16, 33, 45	0
1	C	266/299 (88%)	0.37	20 (7%)	14	11	14, 22, 39, 52	0
2	B	262/269 (97%)	0.10	12 (4%)	32	26	10, 19, 29, 40	0
2	D	269/269 (100%)	0.46	25 (9%)	8	6	11, 23, 38, 45	0
All	All	1093/1136 (96%)	0.26	77 (7%)	16	13	8, 20, 37, 52	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	HIS	7.5
2	D	433	HIS	7.2
1	A	96	LEU	7.2
1	C	253	PRO	6.1
2	D	284	ASP	6.0
2	D	432	VAL	5.8
2	D	434	HIS	5.7
2	B	323	GLN	5.6
2	B	432	VAL	5.4
1	C	296	LEU	5.4
1	A	97	THR	5.2
1	A	38	ASP	5.1
2	D	428	GLU	5.0
2	B	283	ASP	4.9
1	A	36	ARG	4.9
2	D	431	ASN	4.8
1	C	297	ARG	4.8
2	B	171	SER	4.7
1	A	71	HIS	4.7
2	D	285	THR	4.5
2	B	284	ASP	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	171	SER	4.4
2	D	324	PRO	4.3
1	C	287	GLN	4.3
1	C	71[A]	HIS	4.3
2	D	378	GLN	4.2
1	A	74	ASN	4.2
2	D	323	GLN	4.1
2	D	283	ASP	4.1
1	A	73	GLU	4.1
1	C	73[A]	GLU	3.9
1	A	41	THR	3.7
1	A	72	THR	3.6
1	C	269	TYR	3.6
2	B	280	TYR	3.6
2	B	428	GLU	3.4
1	C	36	ARG	3.4
1	C	162	GLU	3.3
1	A	162[A]	GLU	3.3
2	D	439	HIS	3.3
1	C	219	LEU	3.3
2	B	431	ASN	3.2
2	D	280	TYR	2.9
1	A	0	SER	2.8
2	B	285	THR	2.7
2	D	385	GLU	2.6
1	C	2	GLU	2.6
1	C	175	LEU	2.6
1	C	293	VAL	2.6
1	A	95	ALA	2.5
1	A	2	GLU	2.5
2	B	403	GLN	2.4
1	A	19	TYR	2.4
2	D	368	THR	2.4
1	C	216	PHE	2.4
1	A	247	ASP	2.4
1	C	282	ALA	2.3
2	D	400	ARG	2.3
2	D	396	GLN	2.3
1	A	206	ASP	2.3
2	D	436	HIS	2.3
2	D	429	THR	2.3
2	D	365	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	264	SER	2.3
2	B	324	PRO	2.2
1	C	37	LEU	2.2
2	D	327	CYS	2.2
2	D	325	ALA	2.2
1	A	37	LEU	2.2
1	A	297	ARG	2.2
1	C	138	GLU	2.1
2	D	198	GLY	2.1
1	C	38	ASP	2.1
1	A	161	HIS	2.1
1	A	287	GLN	2.1
2	D	430	LEU	2.1
2	B	385	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TPO	A	160	11/12	0.99	0.06	13,14,16,17	0
1	TPO	C	160	11/12	0.99	0.08	16,19,23,23	0

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	SGM	B	1	6/6	0.67	0.40	39,40,41,43	0
4	SGM	B	440	6/6	0.70	0.45	41,41,42,44	0

Continued on next page...

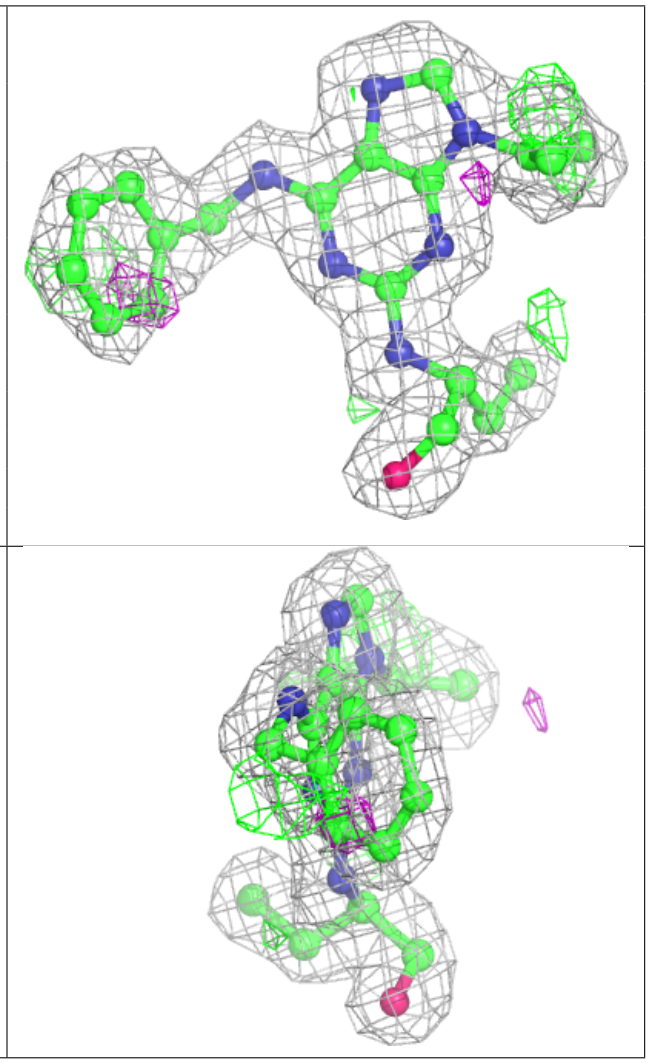
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SGM	D	1	6/6	0.83	0.40	42,44,45,51	0
3	RRC	C	299	26/26	0.89	0.15	16,18,23,24	0
3	RRC	A	299	26/26	0.90	0.15	14,16,21,22	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.

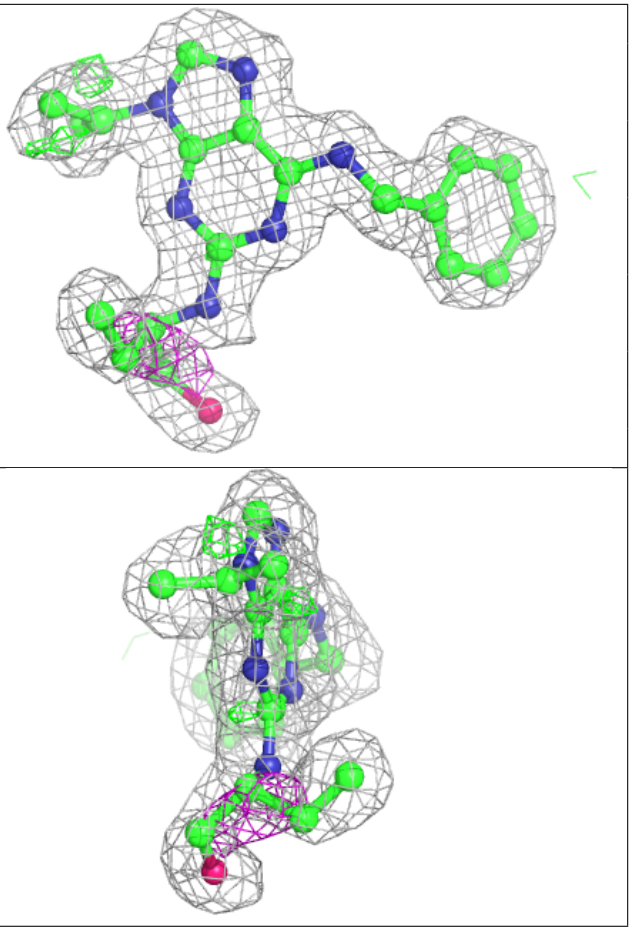
Electron density around RRC C 299:

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 RRC A 299:

$2mF_o$-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.