Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 08:45 pm BST

PDB ID	:	5CYI
Title	:	CDK2/Cyclin A covalent complex with 6-(cyclohexylmethoxy)-N-(4-(vinylsulfonyl)phenyl)-9H-purin-2-amine (NU6300)
Authors	:	Anscombe, E.; Meschini, E.; Vidal, R.M.; Martin, M.P.; Staunton, D.; Geitmann, M.; Danielson, U.H.; Stanley, W.A.; Wang, L.Z.; Reuillon, T.; Golding, B.T.; Cano, C.; Newell, D.R.; Noble, M.E.M.; Wedge, S.R.; Endicott, J.A.; Griffin, R.J.
Deposited on	:	2015-07-30
Resolution	:	2.00 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:

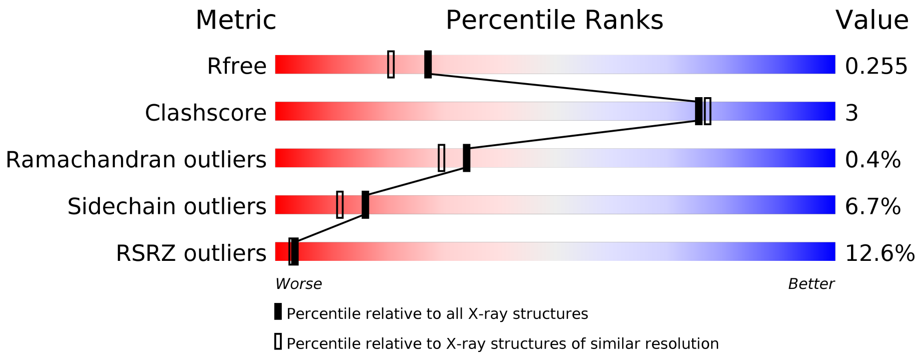
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	303	4% / 82% 13% • ••
1	C	303	21% / 86% 12% •
2	B	260	2% / 91% 6% ••
2	D	260	23% / 91% 7% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9513 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total 2414	C 1567	N 410	O 428	P 1	S 8	0	1	0
1	C	297	Total 2397	C 1555	N 405	O 428	P 1	S 8	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

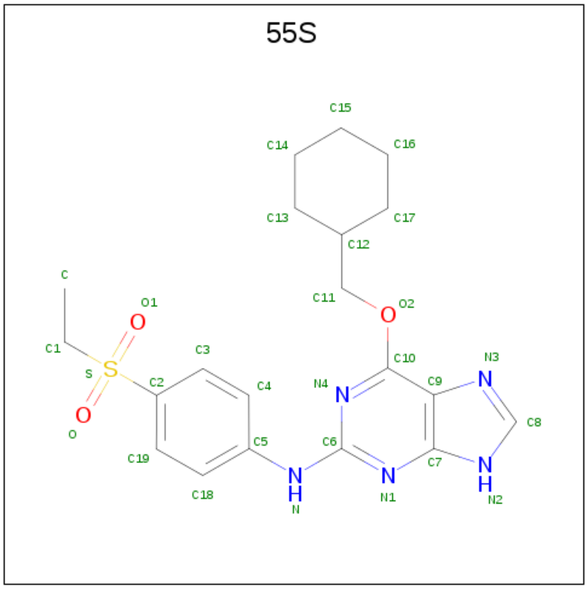
- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total 2083	C 1350	N 339	O 383	S 11	0	0	0
2	D	256	Total 2069	C 1340	N 337	O 381	S 11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	initiating methionine	UNP P20248
D	173	MET	-	initiating methionine	UNP P20248

- Molecule 3 is 6-(cyclohexylmethoxy)-N-[4-(ethylsulfonyl)phenyl]-9H-purin-2-amine (three-letter code: 55S) (formula: $C_{20}H_{25}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 29	C 20	N 5	O 3	S 1	0	0
3	C	1	Total 29	C 20	N 5	O 3	S 1	0	0

- Molecule 4 is water.

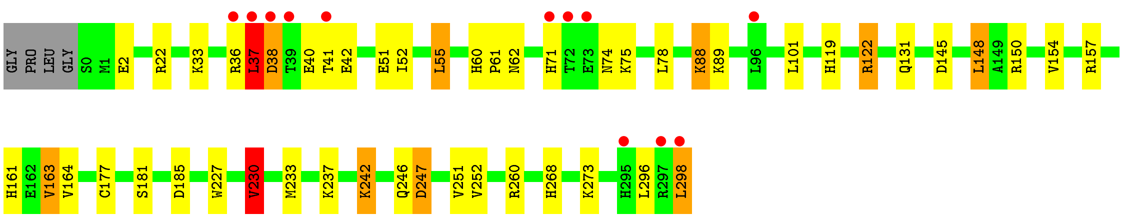
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total 224	O 224	0	0
4	B	166	Total 166	O 166	0	0
4	C	64	Total 64	O 64	0	0
4	D	38	Total 38	O 38	0	0

3 Residue-property plots

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.

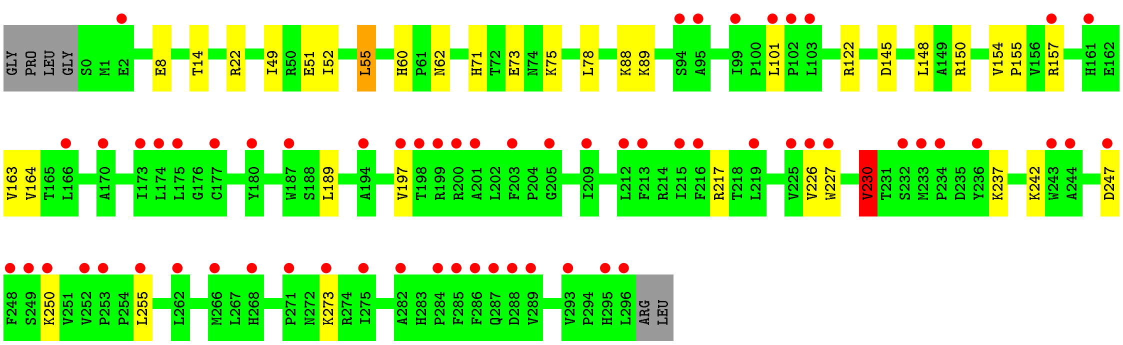
- Molecule 1: Cyclin-dependent kinase 2

Chain A:



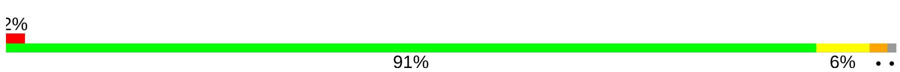
- Molecule 1: Cyclin-dependent kinase 2

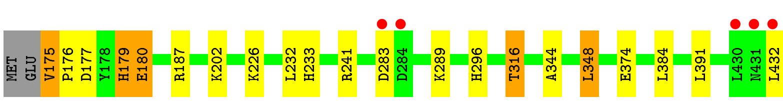
Chain C:



- Molecule 2: Cyclin-A2

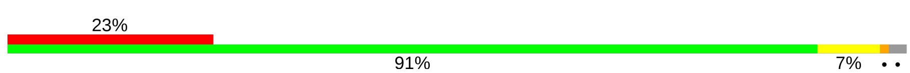
Chain B:

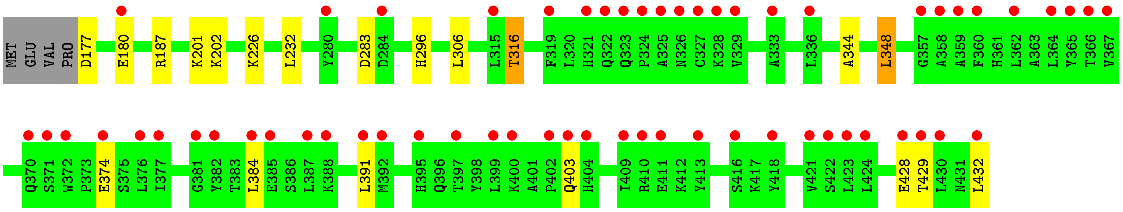




- Molecule 2: Cyclin-A2

Chain D:




MET
GLU
VAL
PRO
D177
E180
R187
K201
K202
K226
L232
Y280
D283
D284
H296
L306
L315
T316
F319
L320
H321
Q322
Q323
P324
A325
N326
C327
K328
V329
A333
L336
A344
L348
G357
A358
A359
F360
H361
L362
A363
L364
Y365
T366
V367
Q370
S371
W372
P373
E374
S375
L376
I377
G381
Y382
T383
L384
E385
S386
L387
K388
L391
M392
H395
Q396
T397
Y398
L399
K400
A401
P402
Q403
H404
I409
R410
E411
K412
Y413
S416
K417
Y418
V421
S422
L423
L424
E428
T429
L430
N431
L432

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.29Å 135.29Å 148.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.34 – 2.00 74.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.34-2.00) 99.9 (74.34-2.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.227 , 0.255 0.227 , 0.255	Depositor DCC
R_{free} test set	4914 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.6	EDS
L-test for twinning[2]	$< \|L\| >= 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9513	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 55S

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	0.74	0/2464	0.97	6/3343 (0.2%)
1	C	0.68	0/2447	0.90	2/3320 (0.1%)
2	B	0.63	1/2133 (0.0%)	0.86	4/2897 (0.1%)
2	D	0.55	0/2118	0.78	2/2875 (0.1%)
All	All	0.66	1/9162 (0.0%)	0.88	14/12435 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	180	GLU	CG-CD	5.00	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	177	ASP	CB-CG-OD1	11.28	128.45	118.30
1	A	38	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	148	LEU	CB-CG-CD2	7.97	124.55	111.00
1	A	37	LEU	CB-CG-CD2	7.96	124.53	111.00
1	C	230	VAL	CB-CA-C	-6.74	98.60	111.40
1	A	230	VAL	CB-CA-C	-6.60	98.87	111.40
2	B	177	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	C	217	ARG	NE-CZ-NH1	5.94	123.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	177	ASP	CB-CG-OD1	5.40	123.16	118.30
2	B	241	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	D	187	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	B	187	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	122	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	247	ASP	CB-CA-C	5.07	120.53	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	GLU	Peptide
1	A	41	THR	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	2414	0	2459	34	0
1	C	2397	0	2432	15	1
2	B	2083	0	2107	12	0
2	D	2069	0	2091	7	1
3	A	29	0	23	0	0
3	C	29	0	24	0	0
4	A	224	0	0	10	0
4	B	166	0	0	4	0
4	C	64	0	0	0	0
4	D	38	0	0	0	0
All	All	9513	0	9136	56	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 3.

All (56) 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:148:LEU:HD22	4:A:497:HOH:O	1.76	0.83
1:A:71:HIS:HD2	2:B:296:HIS:NE2	1.80	0.80
1:A:230:VAL:HA	1:A:233:MET:CE	2.13	0.79
1:A:154:VAL:O	2:B:316:THR:CG2	2.40	0.69
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.59	0.69
1:A:230:VAL:HA	1:A:233:MET:HE2	1.76	0.67
1:A:246:GLN:NE2	4:A:401:HOH:O	2.25	0.65
1:A:242:LYS:HD2	4:A:431:HOH:O	1.97	0.64
1:A:161:HIS:HD2	4:A:607:HOH:O	1.80	0.64
1:C:227:TRP:O	1:C:230:VAL:HG22	2.00	0.62
2:B:316:THR:HG21	4:B:648:HOH:O	1.99	0.61
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.82	0.61
1:A:268:HIS:CD2	4:A:478:HOH:O	2.54	0.60
1:A:230:VAL:HA	1:A:233:MET:HE3	1.84	0.59
1:A:60:HIS:HD2	1:A:62:ASN:H	1.49	0.59
1:C:154:VAL:O	2:D:316:THR:CG2	2.51	0.58
1:A:227:TRP:O	1:A:230:VAL:HG22	2.04	0.57
1:A:296:LEU:HD13	1:A:298:LEU:HD11	1.86	0.57
1:A:60:HIS:CD2	1:A:62:ASN:H	2.23	0.57
1:A:181:SER:HB3	4:A:553:HOH:O	2.04	0.57
1:C:71:HIS:HD2	2:D:296:HIS:NE2	2.02	0.56
1:A:154:VAL:O	2:B:316:THR:HG23	2.05	0.56
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.88	0.55
1:A:119:HIS:HD2	4:B:546:HOH:O	1.89	0.55
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.88	0.55
2:B:176:PRO:HA	2:B:179:HIS:CG	2.42	0.55
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.88	0.54
1:C:60:HIS:CD2	1:C:62:ASN:H	2.27	0.52
1:A:51:GLU:O	1:A:55:LEU:HB2	2.09	0.52
1:C:60:HIS:HD2	1:C:62:ASN:H	1.56	0.52
1:A:154:VAL:O	2:B:316:THR:HG22	2.10	0.52
1:C:51:GLU:O	1:C:55:LEU:HB2	2.11	0.51
1:A:163:VAL:CG2	4:A:497:HOH:O	2.58	0.51
1:C:154:VAL:O	2:D:316:THR:HG22	2.10	0.50
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.47	0.49
2:B:233:HIS:HD2	4:B:607:HOH:O	1.94	0.49
1:A:296:LEU:HD13	1:A:298:LEU:CD1	2.43	0.49
1:A:252:VAL:HB	4:A:403:HOH:O	2.12	0.48
1:A:177:CYS:SG	1:A:233:MET:SD	3.12	0.48
1:A:2:GLU:OE2	1:C:73:GLU:CG	2.61	0.48
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.97	0.47
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:TRP:CE3	1:C:230:VAL:HG13	2.50	0.47
2:B:176:PRO:HA	2:B:179:HIS:CD2	2.51	0.46
2:B:175:VAL:O	2:B:175:VAL:HG13	2.16	0.46
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.98	0.45
1:A:88:LYS:HG2	1:A:131:GLN:NE2	2.32	0.44
1:A:2:GLU:OE2	1:C:73:GLU:HG3	2.17	0.44
1:A:37:LEU:N	1:A:37:LEU:HD13	2.33	0.43
1:A:260:ARG:HD3	4:A:473:HOH:O	2.19	0.43
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.89	0.42
1:A:33:LYS:NZ	4:A:410:HOH:O	2.49	0.42
2:B:289:LYS:HE2	4:B:532:HOH:O	2.21	0.41
1:C:197:VAL:HG21	1:C:255:LEU:HD13	2.02	0.41
1:A:251:VAL:HG12	1:A:252:VAL:HG23	2.03	0.40
1:A:119:HIS:HE1	1:A:185:ASP:OD2	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:C:8:GLU:OE1	2:D:403:GLN:OE1[3_655]	2.18	0.02

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	297/303 (98%)	288 (97%)	7 (2%)	2 (1%)	22	16
1	C	295/303 (97%)	288 (98%)	5 (2%)	2 (1%)	22	16
2	B	256/260 (98%)	255 (100%)	1 (0%)	0	100	100
2	D	254/260 (98%)	253 (100%)	1 (0%)	0	100	100
All	All	1102/1126 (98%)	1084 (98%)	14 (1%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL
1	A	145	ASP
1	C	145	ASP

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	264/265 (100%)	242 (92%)	22 (8%)	11	7
1	C	262/265 (99%)	243 (93%)	19 (7%)	14	9
2	B	232/234 (99%)	219 (94%)	13 (6%)	21	17
2	D	230/234 (98%)	218 (95%)	12 (5%)	23	19
All	All	988/998 (99%)	922 (93%)	66 (7%)	16	11

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	36	ARG
1	A	37	LEU
1	A	38	ASP
1	A	42	GLU
1	A	55	LEU
1	A	61	PRO
1	A	74	ASN
1	A	75	LYS
1	A	88	LYS
1	A	89	LYS
1	A	101	LEU
1	A	122	ARG
1	A	150	ARG
1	A	157	ARG
1	A	163	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	230	VAL
1	A	237	LYS
1	A	242	LYS
1	A	247	ASP
1	A	273	LYS
1	A	298	LEU
2	B	175	VAL
2	B	179	HIS
2	B	180	GLU
2	B	202	LYS
2	B	226	LYS
2	B	232	LEU
2	B	283	ASP
2	B	316	THR
2	B	348	LEU
2	B	374	GLU
2	B	384	LEU
2	B	391	LEU
2	B	432	LEU
1	C	14	THR
1	C	22	ARG
1	C	55	LEU
1	C	75	LYS
1	C	88	LYS
1	C	89	LYS
1	C	101	LEU
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	157	ARG
1	C	163	VAL
1	C	226	VAL
1	C	230	VAL
1	C	237	LYS
1	C	242	LYS
1	C	247	ASP
1	C	250	LYS
1	C	273	LYS
2	D	180	GLU
2	D	201	LYS
2	D	202	LYS
2	D	226	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	232	LEU
2	D	283	ASP
2	D	316	THR
2	D	348	LEU
2	D	374	GLU
2	D	384	LEU
2	D	391	LEU
2	D	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	71	HIS
1	A	119	HIS
1	A	161	HIS
1	A	268	HIS
1	A	272	ASN
2	B	179	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	395	HIS
1	C	59	ASN
1	C	60	HIS
1	C	71	HIS
1	C	119	HIS
2	D	254	GLN
2	D	395	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	C	160	1	8,10,11	1.03	1 (12%)	10,14,16	1.21	1 (10%)
1	TPO	A	160	1	8,10,11	1.45	1 (12%)	10,14,16	1.27	2 (20%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-OG1	3.09	1.65	1.59
1	C	160	TPO	P-OG1	2.22	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TPO	O3P-P-O1P	2.74	121.39	110.68
1	A	160	TPO	O3P-P-O1P	2.26	119.51	110.68
1	A	160	TPO	O-C-CA	-2.06	119.39	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	55S	A	301	1	29,32,32	1.07	1 (3%)	36,45,45	0.78	2 (5%)
3	55S	C	301	1	29,32,32	0.91	2 (6%)	36,45,45	0.69	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
3	55S	A	301	1	-	3/18/26/26	0/4/4/4
3	55S	C	301	1	-	5/18/26/26	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	55S	O2-C10	4.51	1.38	1.35
3	C	301	55S	O2-C10	3.00	1.37	1.35
3	C	301	55S	C5-N	2.12	1.45	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	55S	C6-N4-C10	2.23	119.12	115.18
3	A	301	55S	C-C1-S	2.16	116.99	112.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

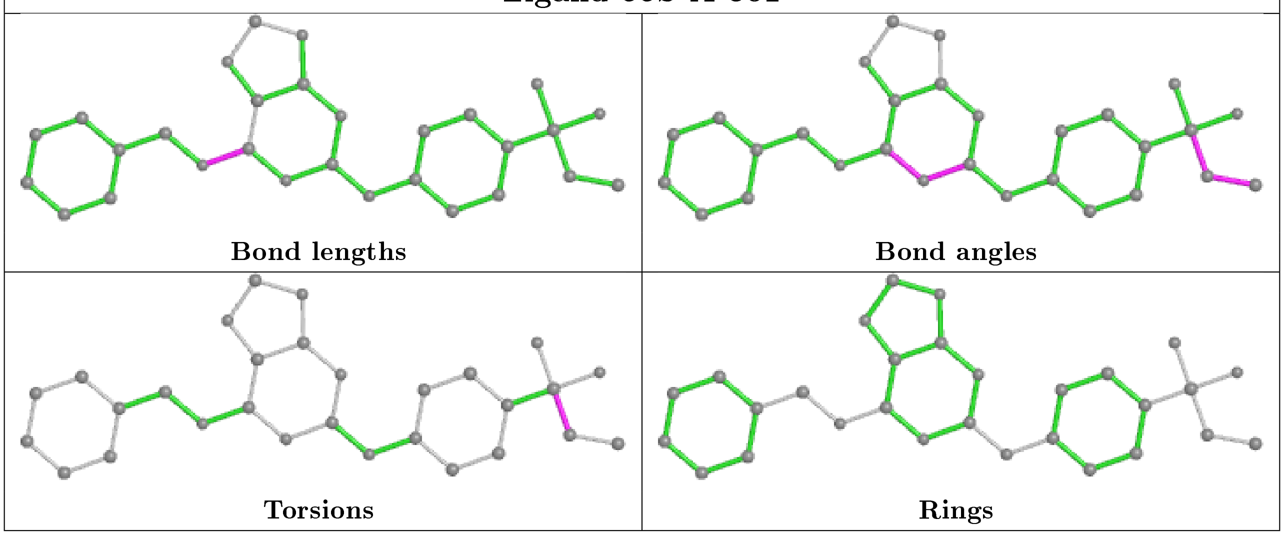
Mol	Chain	Res	Type	Atoms
3	A	301	55S	C-C1-S-O1
3	A	301	55S	C-C1-S-O
3	A	301	55S	C-C1-S-C2
3	C	301	55S	C-C1-S-O1
3	C	301	55S	C-C1-S-O
3	C	301	55S	C-C1-S-C2
3	C	301	55S	N1-C6-N-C5
3	C	301	55S	N4-C6-N-C5

There are no ring outliers.

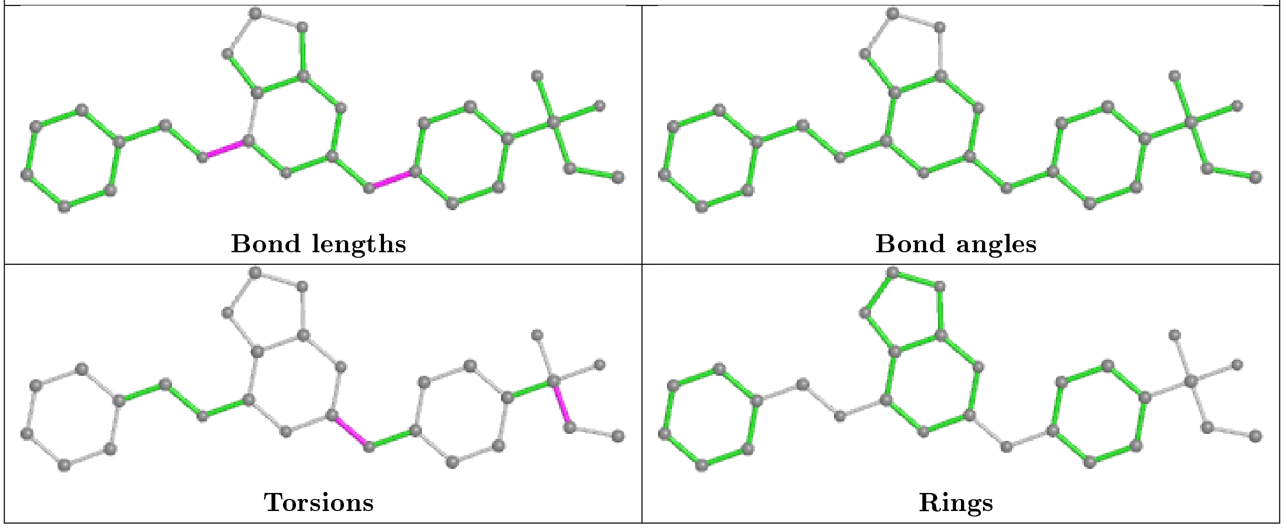
No monomer is involved in short contacts.

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 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 55S A 301



Ligand 55S C 301



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	298/303 (98%)	0.51	12 (4%)	38	37	20, 32, 76, 119	0
1	C	296/303 (97%)	1.09	63 (21%)	0	0	34, 62, 96, 118	0
2	B	258/260 (99%)	0.09	5 (1%)	66	65	22, 34, 63, 118	0
2	D	256/260 (98%)	1.22	60 (23%)	0	0	31, 69, 118, 139	0
All	All	1108/1126 (98%)	0.73	140 (12%)	3	3	20, 46, 100, 139	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	372	TRP	8.2
1	C	296	LEU	7.6
2	D	327	CYS	7.5
2	D	399	LEU	6.5
2	D	324	PRO	6.0
2	D	423	LEU	6.0
1	A	96	LEU	5.9
1	C	225	VAL	5.8
2	D	430	LEU	5.7
1	C	101	LEU	5.3
2	D	328	LYS	5.2
1	C	236	TYR	5.2
1	C	173	ILE	4.9
1	C	213	PHE	4.8
2	D	323	GLN	4.8
2	D	329	VAL	4.7
1	C	99	ILE	4.7
2	D	284	ASP	4.6
2	B	431	ASN	4.5
1	C	253	PRO	4.4
2	D	367	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	384	LEU	4.3
1	C	197	VAL	4.3
1	C	252	VAL	4.3
1	C	255	LEU	4.2
1	C	215	ILE	4.1
2	D	366	THR	4.1
2	D	364	LEU	4.1
1	A	73	GLU	4.0
1	C	248	PHE	4.0
2	D	359	ALA	4.0
1	C	282	ALA	4.0
1	C	249	SER	3.9
2	D	403	GLN	3.9
2	D	333	ALA	3.8
2	B	432	LEU	3.8
2	D	418	TYR	3.7
2	D	374	GLU	3.7
1	C	209	ILE	3.6
1	A	298	LEU	3.6
1	C	295	HIS	3.6
1	C	286	PHE	3.6
2	D	413	TYR	3.6
1	C	243	TRP	3.6
1	C	287	GLN	3.5
2	D	325	ALA	3.5
1	C	199	ARG	3.4
2	D	321	HIS	3.4
2	D	395	HIS	3.4
1	A	295	HIS	3.4
1	A	72	THR	3.3
1	C	219	LEU	3.3
2	B	284	ASP	3.2
2	D	326	ASN	3.2
1	A	297	ARG	3.1
2	D	428	GLU	3.1
1	C	284	PRO	3.1
1	A	39	THR	3.1
2	D	388	LYS	3.0
1	A	37	LEU	3.0
1	C	200	ARG	3.0
1	C	271	PRO	3.0
2	D	429	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	212	LEU	3.0
2	D	280	TYR	2.9
1	C	94	SER	2.9
2	D	400	LYS	2.9
1	C	226	VAL	2.9
1	C	293	VAL	2.9
2	D	382	TYR	2.9
1	C	262	LEU	2.9
2	D	336	LEU	2.9
2	D	397	THR	2.8
1	C	187	TRP	2.8
1	C	233	MET	2.8
2	D	392	MET	2.8
1	C	250	LYS	2.8
1	C	216	PHE	2.8
1	C	268	HIS	2.8
1	C	157	ARG	2.8
1	C	247	ASP	2.8
2	D	315	LEU	2.8
2	D	424	LEU	2.7
2	D	365	TYR	2.7
2	D	402	PRO	2.7
2	D	421	VAL	2.7
1	A	36	ARG	2.7
2	D	391	LEU	2.7
1	C	170	ALA	2.6
2	D	422	SER	2.6
2	D	360	PHE	2.6
1	C	227	TRP	2.6
1	C	180	TYR	2.5
2	D	319	PHE	2.5
1	A	71	HIS	2.5
1	C	285	PHE	2.5
1	C	273	LYS	2.5
2	D	371	SER	2.5
2	D	409	ILE	2.5
2	D	416	SER	2.5
2	D	387	LEU	2.4
1	A	38	ASP	2.4
2	D	385	GLU	2.4
1	C	102	PRO	2.4
1	C	166	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	357	GLY	2.4
1	C	203	PHE	2.4
1	C	289	VAL	2.4
2	D	370	GLN	2.4
2	D	411	GLU	2.3
1	C	198	THR	2.3
2	D	322	GLN	2.3
1	C	288	ASP	2.3
1	C	174	LEU	2.2
1	C	175	LEU	2.2
2	D	358	ALA	2.2
1	C	232	SER	2.2
1	C	234	PRO	2.2
2	D	432	LEU	2.2
1	C	266	MET	2.2
1	C	95	ALA	2.2
1	C	194	ALA	2.2
2	D	180	GLU	2.2
2	B	430	LEU	2.1
1	C	177	CYS	2.1
2	D	376	LEU	2.1
1	C	205	GLY	2.1
1	A	41	THR	2.1
1	C	244	ALA	2.1
1	C	161	HIS	2.1
1	C	275	ILE	2.1
2	D	377	ILE	2.1
1	C	103	LEU	2.1
1	C	2	GLU	2.1
2	D	381	GLY	2.1
2	D	362	LEU	2.1
2	B	283	ASP	2.0
1	C	201	ALA	2.0
2	D	404	HIS	2.0
2	D	410	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	C	160	11/12	0.93	0.13	45,59,67,70	0
1	TPO	A	160	11/12	0.99	0.12	22,27,29,29	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

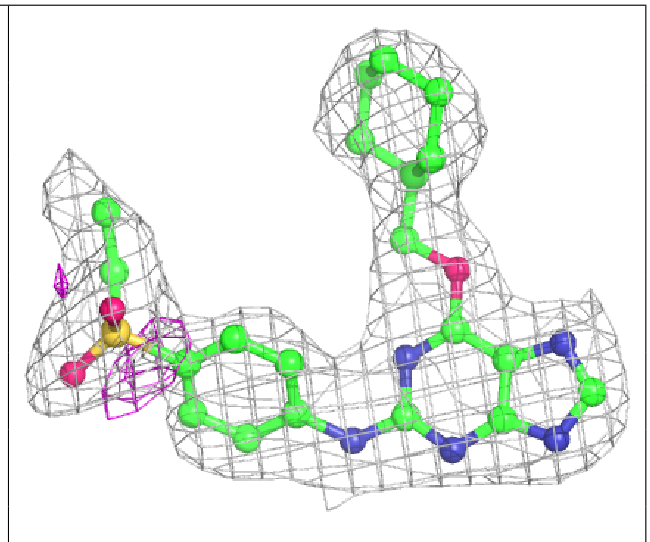
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

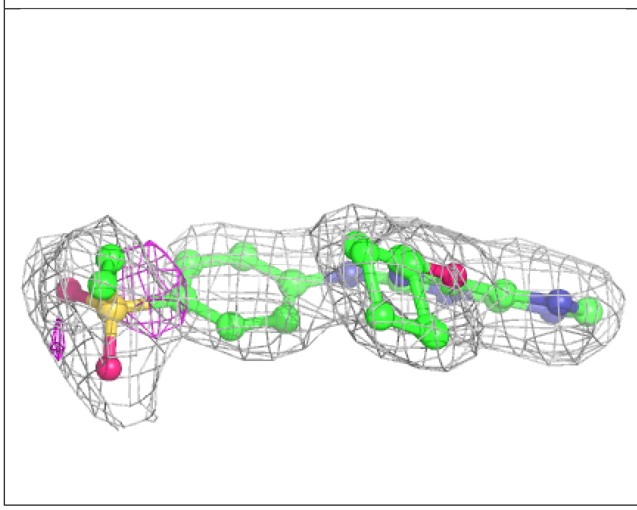
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	55S	C	301	29/29	0.94	0.13	38,48,64,72	0
3	55S	A	301	29/29	0.96	0.12	35,40,63,67	0

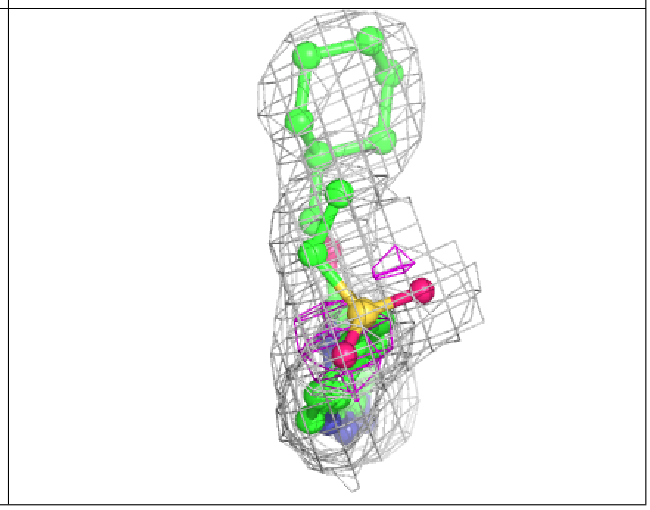
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 55S C 301:

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

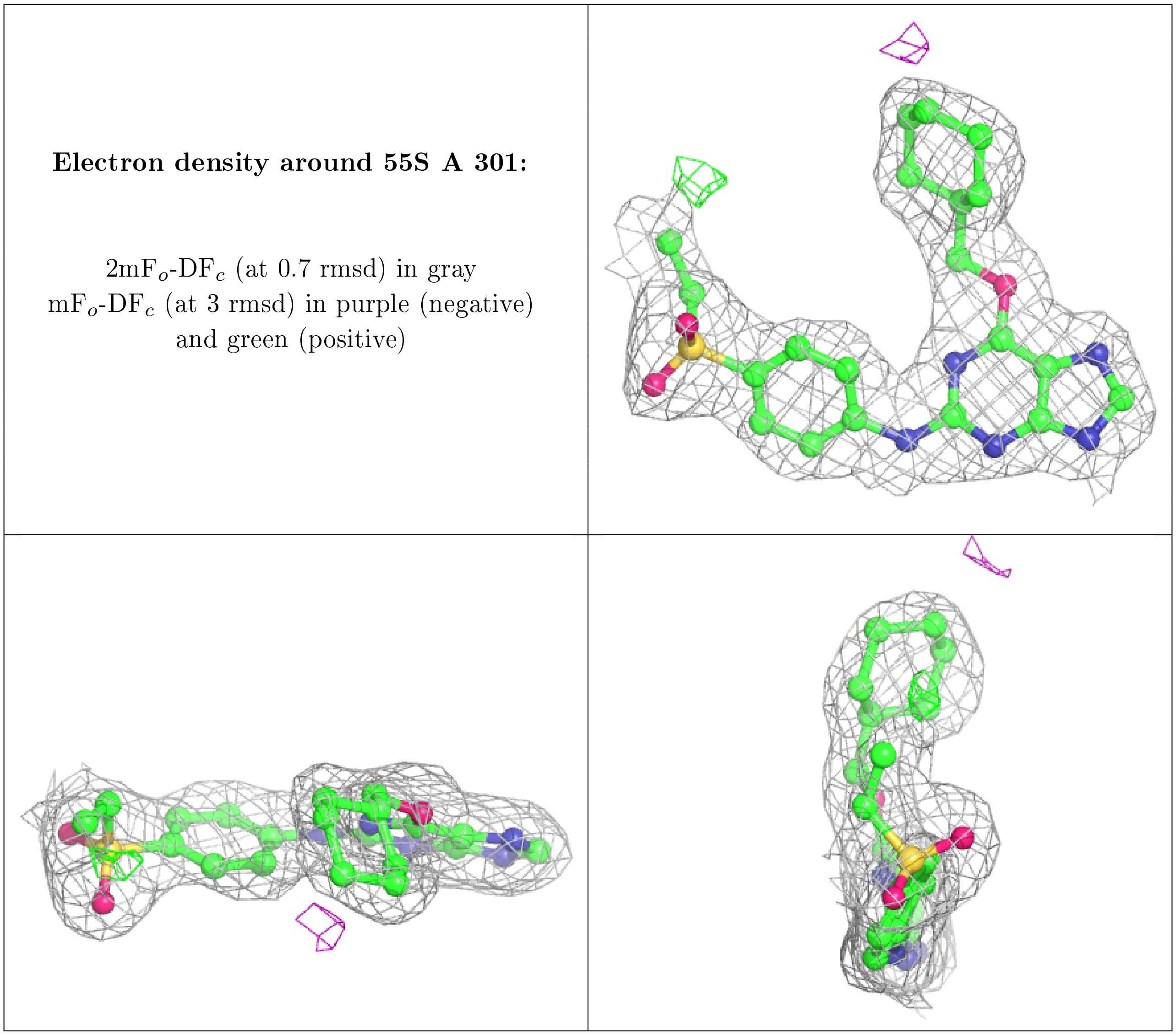






Electron density around 55S A 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.