Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 10:16 AM EDT

PDB ID	:	1OPL
Title	:	Structural basis for the auto-inhibition of c-Abl tyrosine kinase
Authors	:	Nagar, B.; Hantschel, O.; Young, M.A.; Scheffzek, K.; Veach, D.; Bornmann, W.; Clarkson, B.; Superti-Furga, G.; Kuriyan, J.
Deposited on	:	2003-03-06
Resolution	:	3.42 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:

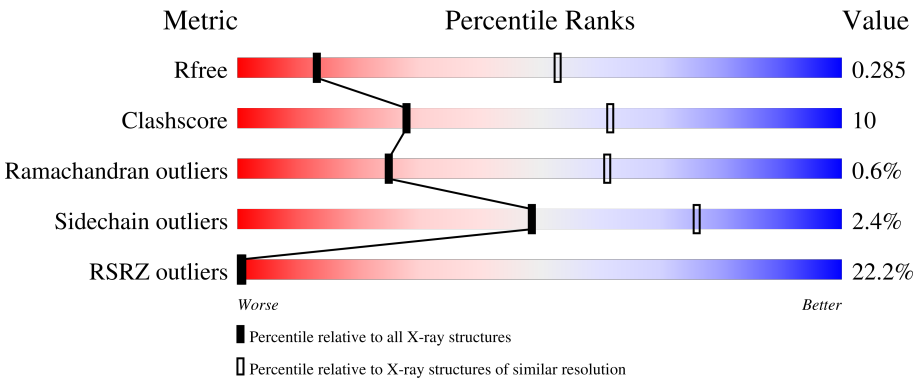
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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	537	4%, 72%, 11%, •, 16%
1	B	537	30%, 53%, 14%, •, 32%

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	MYR	A	538	-	-	-	X
3	P16	B	538	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6655 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.

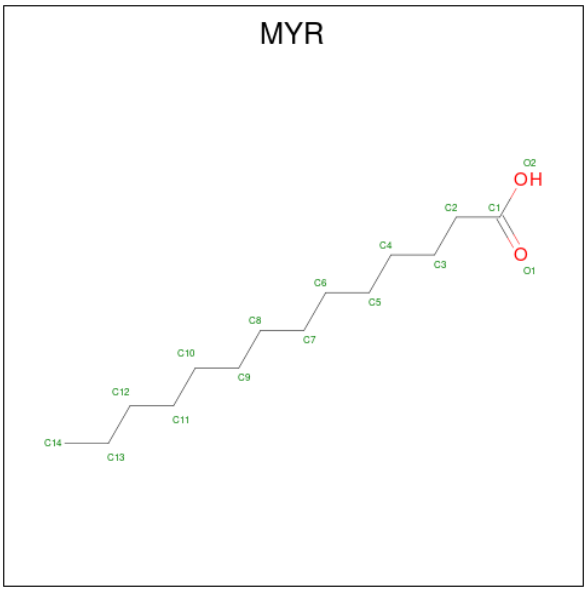
- Molecule 1 is a protein called proto-oncogene tyrosine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	451	3628	2314	611	685	18	0	0	0
1	B	365	2954	1889	497	551	17	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

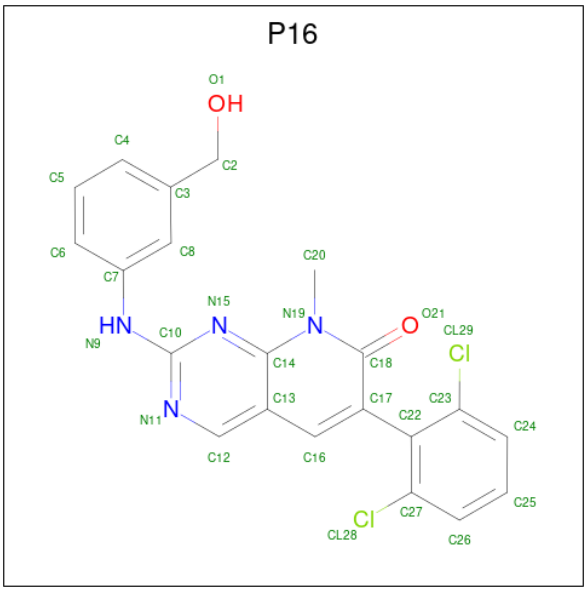
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ARG	LYS	engineered mutation	UNP P00519
A	30	ASP	GLU	engineered mutation	UNP P00519
A	382	ASN	ASP	engineered mutation	UNP P00519
A	532	GLU	-	cloning artifact	UNP P00519
A	533	ASN	-	cloning artifact	UNP P00519
A	534	LEU	-	cloning artifact	UNP P00519
A	535	TYR	-	cloning artifact	UNP P00519
A	536	PHE	-	cloning artifact	UNP P00519
A	537	GLN	-	cloning artifact	UNP P00519
B	29	ARG	LYS	engineered mutation	UNP P00519
B	30	ASP	GLU	engineered mutation	UNP P00519
B	382	ASN	ASP	engineered mutation	UNP P00519
B	532	GLU	-	cloning artifact	UNP P00519
B	533	ASN	-	cloning artifact	UNP P00519
B	534	LEU	-	cloning artifact	UNP P00519
B	535	TYR	-	cloning artifact	UNP P00519
B	536	PHE	-	cloning artifact	UNP P00519
B	537	GLN	-	cloning artifact	UNP P00519

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	15	14	1	0	0

- Molecule 3 is 6-(2,6-DICHLOROPHENYL)-2-{[3-(HYDROXYMETHYL)PHENYL]AMINO}-8-METHYLPYRIDO[2,3-D]PYRIMIDIN-7(8H)-ONE (three-letter code: P16) (formula: $C_{21}H_{16}Cl_2N_4O_2$).



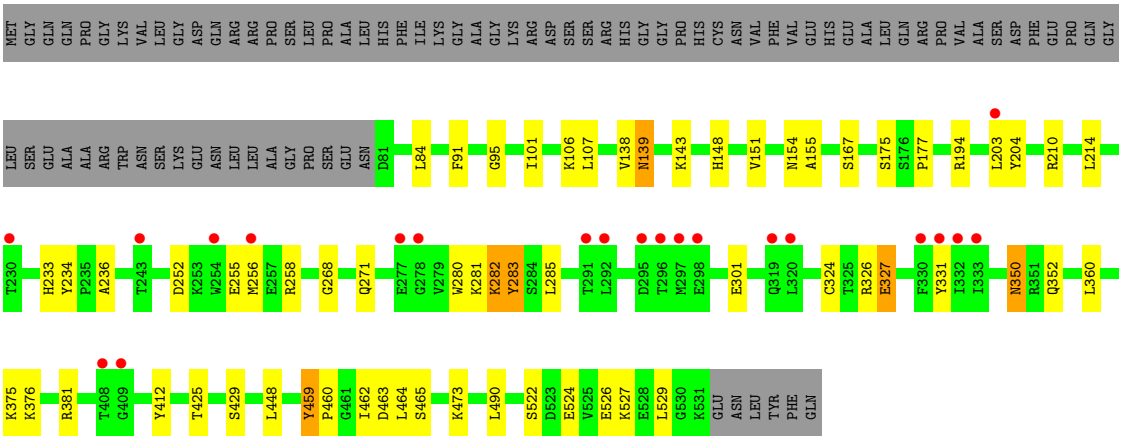
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	29	21	2	4	2	0	0
			Total	C	Cl	N	O		
3	B	1	29	21	2	4	2	0	0

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.

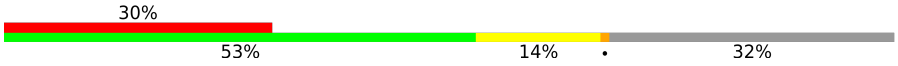
• Molecule 1: proto-oncogene tyrosine-protein kinase

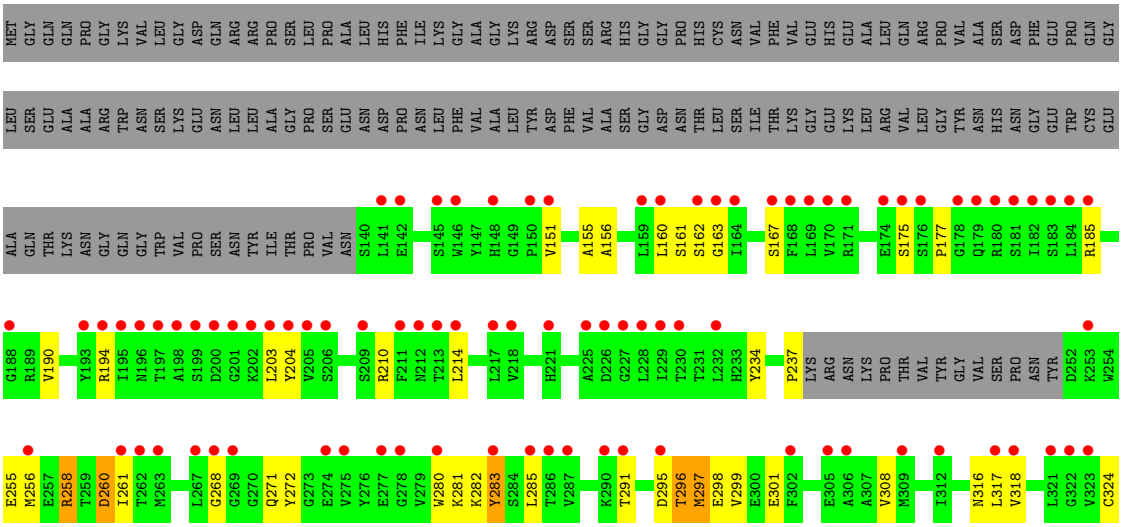
Chain A:

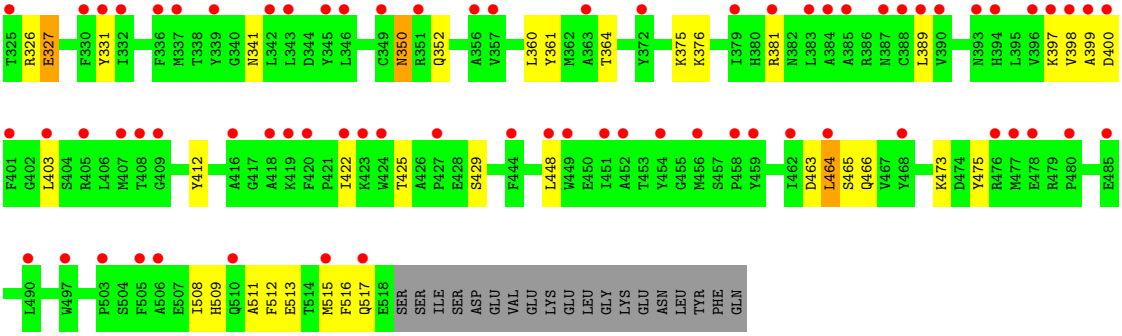


• Molecule 1: proto-oncogene tyrosine-protein kinase

Chain B:






T325
R326
E327
F330
Y331
I332
F336
M337
T338
Y339
G340
N341
L342
L343
D344
Y345
L346
C349
N350
R351
Q352
A356
V357
L360
Y361
M362
A363
T364
Y372
K375
K376
I379
H380
R381
N382
L383
A384
A385
R386
N387
C388
L389
V390
N393
H394
L395
V396
K397
V398
A399
D400
F401
G402
L403
S404
R405
L406
M407
T408
G409
Y412
A416
G417
A418
K419
F420
P421
I422
K423
W424
T425
A426
P427
E428
S429
F444
L448
W449
E450
I451
A452
T453
Y454
G455
M456
S457
P458
Y459
I462
D463
L464
S465
Q466
V467
Y468
K473
D474
Y475
R476
M477
E478
R479
P480
E485
L490
W497
P503
S504
F505
A506
E507
I508
H509
Q510
A511
F512
E513
T514
M515
F516
Q517
E518
SER
SER
ILE
SER
ASP
GLU
VAL
GLU
LYS
GLU
LEU
GLY
LYS
GLU
ASN
LEU
TYR
PHE
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	77.02Å 273.38Å 124.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.42 74.13 – 3.42	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.95-3.42) 89.2 (74.13-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 3.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.306 , 0.315 0.270 , 0.285	Depositor DCC
R_{free} test set	1110 reflections (6.84%)	wwPDB-VP
Wilson B-factor (Å^2)	102.4	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 90.7	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	0.89	EDS
Total number of atoms	6655	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: MYR, P16

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	0.48	1/3723 (0.0%)	0.71	3/5049 (0.1%)
1	B	0.53	0/3031	0.77	2/4105 (0.0%)
All	All	0.50	1/6754 (0.0%)	0.74	5/9154 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	460	PRO	N-CD	5.29	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	464	LEU	CB-CA-C	6.88	123.28	110.20
1	A	95	GLY	N-CA-C	-6.14	97.75	113.10
1	A	459	TYR	CB-CG-CD1	6.11	124.66	121.00
1	B	234	TYR	N-CA-CB	-5.47	100.76	110.60
1	A	459	TYR	CB-CG-CD2	-5.05	117.97	121.00

There are no chirality outliers.

There are no planarity outliers.

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	3628	0	3525	46	0
1	B	2954	0	2875	86	0
2	A	15	0	27	3	0
3	A	29	0	16	1	0
3	B	29	0	16	3	0
All	All	6655	0	6459	130	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 10.

All (130) 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:529:LEU:HD11	2:A:538:MYR:H42	1.55	0.88
1:B:162:SER:HB2	1:B:258:ARG:HG3	1.59	0.82
1:B:360:LEU:HD21	1:B:516:PHE:HA	1.61	0.80
1:B:360:LEU:CD2	1:B:516:PHE:HA	2.10	0.80
1:B:399:ALA:HB1	3:B:538:P16:CL28	2.21	0.77
1:B:258:ARG:NH1	1:B:258:ARG:HB3	2.03	0.73
1:A:139:ASN:H	1:A:139:ASN:HD22	1.35	0.72
1:A:84:LEU:HD21	1:A:106:LYS:HD3	1.74	0.70
1:B:316:ASN:HA	1:B:397:LYS:HG2	1.73	0.69
1:B:422:ILE:HB	1:B:464:LEU:HD13	1.76	0.67
1:B:258:ARG:HB3	1:B:258:ARG:CZ	2.24	0.67
1:B:295:ASP:O	1:B:296:THR:HB	1.95	0.66
1:B:258:ARG:O	1:B:258:ARG:HG2	1.97	0.64
1:B:296:THR:HG23	1:B:297:MET:N	2.13	0.64
1:B:295:ASP:OD1	1:B:296:THR:N	2.30	0.64
1:A:203:LEU:HD12	1:A:203:LEU:N	2.13	0.64
1:B:162:SER:CB	1:B:258:ARG:HG3	2.28	0.63
1:B:509:HIS:O	1:B:512:PHE:N	2.32	0.63
1:B:203:LEU:HD12	1:B:203:LEU:N	2.13	0.63
1:B:318:VAL:CG2	1:B:389:LEU:HD12	2.29	0.63
1:B:318:VAL:HG21	1:B:389:LEU:HD12	1.80	0.62
1:B:185:ARG:HH11	1:B:190:VAL:CG2	2.11	0.61
1:B:175:SER:O	1:B:177:PRO:HD3	2.01	0.61
1:A:522:SER:O	1:A:526:GLU:HG2	2.01	0.61
1:B:360:LEU:HD21	1:B:516:PHE:CA	2.31	0.60
1:A:175:SER:O	1:A:177:PRO:HD3	2.01	0.60
1:B:258:ARG:O	1:B:258:ARG:CG	2.50	0.60
1:B:185:ARG:HD2	1:B:190:VAL:HG22	1.84	0.59
1:B:364:THR:HG23	1:B:512:PHE:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:O	1:B:397:LYS:HA	2.03	0.58
1:A:473:LYS:O	1:B:473:LYS:HE2	2.05	0.57
1:B:156:ALA:O	1:B:160:LEU:HB2	2.04	0.57
1:B:163:GLY:HA3	1:B:167:SER:CB	2.35	0.57
1:B:509:HIS:C	1:B:511:ALA:N	2.59	0.56
1:B:463:ASP:N	1:B:463:ASP:OD1	2.39	0.55
1:A:473:LYS:HE2	1:B:475:TYR:HB2	1.87	0.55
1:B:508:ILE:O	1:B:511:ALA:HB3	2.07	0.55
1:B:517:GLN:NE2	1:B:517:GLN:HA	2.22	0.55
1:B:185:ARG:NH1	1:B:190:VAL:HG23	2.22	0.54
1:B:360:LEU:HD21	1:B:515:MET:C	2.28	0.54
1:A:529:LEU:HD11	2:A:538:MYR:C4	2.33	0.54
1:B:151:VAL:HG13	1:B:155:ALA:HB3	1.91	0.53
1:B:517:GLN:HA	1:B:517:GLN:HE21	1.73	0.53
1:A:350:ASN:HD21	1:A:352:GLN:HG2	1.74	0.53
1:B:258:ARG:C	1:B:260:ASP:H	2.10	0.53
1:B:295:ASP:OD1	1:B:295:ASP:C	2.45	0.53
1:B:350:ASN:HD21	1:B:352:GLN:HG2	1.74	0.53
1:A:167:SER:HA	1:A:234:TYR:HB2	1.91	0.52
1:A:360:LEU:HA	2:A:538:MYR:H142	1.91	0.52
1:B:361:TYR:CD1	1:B:516:PHE:CZ	2.97	0.52
1:A:151:VAL:HG13	1:A:155:ALA:HB3	1.91	0.52
1:B:308:VAL:HG11	1:B:403:LEU:HB2	1.92	0.50
1:A:194:ARG:HB2	1:A:194:ARG:NH1	2.28	0.49
1:B:194:ARG:NH1	1:B:194:ARG:HB2	2.28	0.49
1:A:139:ASN:CG	1:A:139:ASN:O	2.51	0.49
1:B:258:ARG:CZ	1:B:258:ARG:CB	2.90	0.48
1:A:154:ASN:ND2	1:A:360:LEU:HD21	2.27	0.48
1:A:280:TRP:CE2	1:A:283:TYR:HE1	2.32	0.48
1:B:324:CYS:HB2	1:B:331:TYR:HB2	1.95	0.48
1:A:91:PHE:HB3	1:A:101:ILE:HG12	1.96	0.48
1:B:280:TRP:CE2	1:B:283:TYR:HE1	2.32	0.48
1:A:324:CYS:HB2	1:A:331:TYR:HB2	1.95	0.48
1:B:513:GLU:O	1:B:517:GLN:HG2	2.13	0.48
1:A:167:SER:HA	1:A:234:TYR:O	2.13	0.47
1:B:317:LEU:HD22	1:B:400:ASP:HB3	1.96	0.47
1:B:185:ARG:HH11	1:B:190:VAL:HG23	1.78	0.47
1:B:361:TYR:HD1	1:B:516:PHE:CZ	2.32	0.47
1:B:296:THR:O	1:B:297:MET:C	2.53	0.47
3:A:539:P16:H6	3:A:539:P16:N15	2.30	0.47
1:B:255:GLU:HG3	1:B:326:ARG:NH2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HA	1:B:160:LEU:HD23	1.64	0.46
1:B:326:ARG:C	1:B:327:GLU:HG3	2.35	0.46
1:A:258:ARG:HH11	1:A:258:ARG:HB3	1.81	0.46
1:B:237:PRO:HG2	1:B:258:ARG:CZ	2.45	0.46
1:A:381:ARG:NH1	1:A:412:TYR:HE2	2.14	0.46
1:B:301:GLU:HA	1:B:301:GLU:OE1	2.16	0.46
3:B:538:P16:N15	3:B:538:P16:H6	2.31	0.46
1:A:473:LYS:HE2	1:B:475:TYR:CA	2.46	0.45
1:B:399:ALA:CB	3:B:538:P16:CL28	2.97	0.45
1:A:255:GLU:HG3	1:A:326:ARG:NH2	2.31	0.45
1:A:283:TYR:HB2	1:A:285:LEU:HB2	1.99	0.45
1:A:463:ASP:C	1:A:465:SER:H	2.19	0.45
1:A:473:LYS:HB3	1:B:473:LYS:HD3	1.97	0.45
1:B:272:TYR:OH	1:B:341:ASN:ND2	2.40	0.45
1:B:360:LEU:HD21	1:B:516:PHE:N	2.31	0.45
1:B:364:THR:HG23	1:B:512:PHE:CB	2.47	0.45
1:B:283:TYR:HB2	1:B:285:LEU:HB2	1.99	0.44
1:B:361:TYR:HB2	1:B:516:PHE:CE1	2.52	0.44
1:A:280:TRP:HE1	1:A:282:LYS:HD3	1.82	0.44
1:A:258:ARG:CB	1:A:258:ARG:NH1	2.80	0.44
1:B:381:ARG:NH1	1:B:412:TYR:HE2	2.14	0.44
1:A:524:GLU:OE1	1:A:527:LYS:HE2	2.18	0.44
1:A:301:GLU:HA	1:A:301:GLU:OE1	2.18	0.44
1:B:185:ARG:HD2	1:B:190:VAL:CG2	2.47	0.44
1:A:327:GLU:N	1:A:327:GLU:OE1	2.51	0.43
1:B:317:LEU:HD23	1:B:398:VAL:O	2.18	0.43
1:A:268:GLY:O	1:A:271:GLN:HG2	2.18	0.43
1:B:268:GLY:O	1:B:271:GLN:HG2	2.18	0.43
1:B:463:ASP:O	1:B:465:SER:N	2.51	0.43
1:A:148:HIS:NE2	1:A:236:ALA:O	2.52	0.43
1:B:256:MET:SD	1:B:324:CYS:SG	3.17	0.43
1:B:203:LEU:N	1:B:203:LEU:CD1	2.81	0.43
1:A:375:LYS:HE2	1:A:376:LYS:HE2	2.01	0.43
1:B:375:LYS:HE2	1:B:376:LYS:HE2	2.01	0.43
1:A:203:LEU:N	1:A:203:LEU:CD1	2.81	0.42
1:A:459:TYR:HB3	1:A:462:ILE:HD12	2.01	0.42
1:B:204:TYR:HB3	1:B:210:ARG:HG2	2.01	0.42
1:B:291:THR:O	1:B:291:THR:HG23	2.18	0.42
1:B:283:TYR:CD1	1:B:283:TYR:N	2.87	0.42
1:B:317:LEU:HD23	1:B:398:VAL:HB	2.02	0.42
1:A:283:TYR:CD1	1:A:283:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:SD	1:A:324:CYS:SG	3.18	0.41
1:A:138:VAL:O	1:A:143:LYS:HD3	2.19	0.41
1:B:163:GLY:HA3	1:B:167:SER:HB2	2.02	0.41
1:A:204:TYR:HB3	1:A:210:ARG:HG2	2.01	0.41
1:B:256:MET:HE1	1:B:261:ILE:HG12	2.01	0.41
1:A:425:THR:CG2	1:A:429:SER:HB2	2.51	0.41
1:B:283:TYR:C	1:B:285:LEU:N	2.73	0.41
1:B:299:VAL:H	1:B:299:VAL:HG23	1.55	0.41
1:B:425:THR:CG2	1:B:429:SER:HB2	2.51	0.41
1:A:281:LYS:O	1:A:283:TYR:N	2.54	0.41
1:B:161:SER:HA	1:B:185:ARG:NH1	2.35	0.41
1:A:326:ARG:C	1:A:327:GLU:HG3	2.39	0.41
1:B:281:LYS:O	1:B:283:TYR:N	2.54	0.41
1:A:464:LEU:HD23	1:A:464:LEU:HA	1.67	0.40
1:B:509:HIS:O	1:B:511:ALA:N	2.55	0.40
1:A:194:ARG:HB2	1:A:194:ARG:HH11	1.87	0.40
1:B:194:ARG:HB2	1:B:194:ARG:HH11	1.87	0.40
1:B:466:GLN:HA	1:B:466:GLN:OE1	2.22	0.40
1:B:161:SER:HA	1:B:185:ARG:CZ	2.52	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	449/537 (84%)	430 (96%)	17 (4%)	2 (0%)	34 69
1	B	361/537 (67%)	337 (93%)	21 (6%)	3 (1%)	19 56
All	All	810/1074 (75%)	767 (95%)	38 (5%)	5 (1%)	25 61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	LYS
1	A	252	ASP
1	B	282	LYS
1	B	296	THR
1	B	298	GLU

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	393/463 (85%)	384 (98%)	9 (2%)	50	77
1	B	318/463 (69%)	310 (98%)	8 (2%)	47	75
All	All	711/926 (77%)	694 (98%)	17 (2%)	49	76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LEU
1	A	139	ASN
1	A	214	LEU
1	A	233	HIS
1	A	283	TYR
1	A	327	GLU
1	A	350	ASN
1	A	448	LEU
1	A	490	LEU
1	B	214	LEU
1	B	258	ARG
1	B	260	ASP
1	B	283	TYR
1	B	297	MET
1	B	327	GLU
1	B	350	ASN
1	B	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	233	HIS
1	A	240	ASN
1	A	350	ASN
1	A	393	ASN
1	B	350	ASN
1	B	509	HIS
1	B	517	GLN

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)

3 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	P16	A	539	-	30,32,32	2.09	11 (36%)	36,46,46	1.13	4 (11%)
3	P16	B	538	-	30,32,32	2.08	10 (33%)	36,46,46	1.14	4 (11%)
2	MYR	A	538	-	14,14,15	0.57	0	13,13,15	0.59	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	P16	A	539	-	-	0/6/10/10	0/4/4/4
3	P16	B	538	-	-	0/6/10/10	0/4/4/4
2	MYR	A	538	-	-	5/11/12/13	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	539	P16	C17-C18	5.51	1.51	1.41
3	B	538	P16	C17-C18	5.46	1.51	1.41
3	B	538	P16	C18-N19	4.25	1.44	1.38
3	A	539	P16	C18-N19	4.22	1.44	1.38
3	A	539	P16	C26-C27	3.37	1.43	1.36
3	B	538	P16	C26-C27	3.33	1.43	1.36
3	A	539	P16	C24-C23	3.13	1.43	1.36
3	B	538	P16	C24-C23	3.11	1.43	1.36
3	B	538	P16	C10-N11	3.02	1.38	1.34
3	A	539	P16	C10-N11	3.02	1.38	1.34
3	B	538	P16	C8-C7	2.81	1.44	1.39
3	A	539	P16	C6-C7	2.76	1.43	1.39
3	B	538	P16	C6-C7	2.74	1.43	1.39
3	A	539	P16	C8-C7	2.73	1.43	1.39
3	B	538	P16	C4-C3	2.59	1.44	1.38
3	A	539	P16	C4-C3	2.56	1.44	1.38
3	B	538	P16	C16-C13	2.28	1.43	1.39
3	A	539	P16	C16-C13	2.26	1.43	1.39
3	A	539	P16	C5-C6	2.07	1.43	1.38
3	A	539	P16	C13-C14	2.06	1.45	1.41
3	B	538	P16	C13-C14	2.04	1.45	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	538	P16	C27-C22-C23	-3.33	117.78	125.49
3	A	539	P16	C27-C22-C23	-3.30	117.85	125.49
3	B	538	P16	C10-N15-C14	3.08	118.77	115.28
3	A	539	P16	C10-N15-C14	3.06	118.75	115.28
3	B	538	P16	N11-C10-N15	-2.25	124.35	126.52
3	A	539	P16	N11-C10-N15	-2.21	124.38	126.52
3	A	539	P16	C13-C14-N15	-2.04	120.71	123.37
3	B	538	P16	C13-C14-N15	-2.03	120.73	123.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

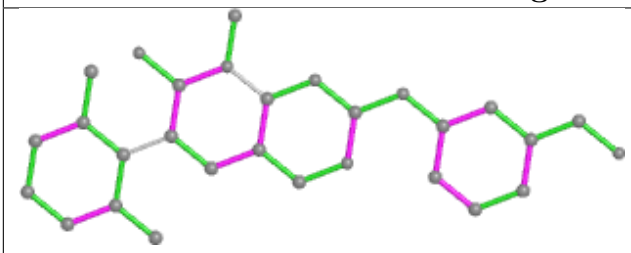
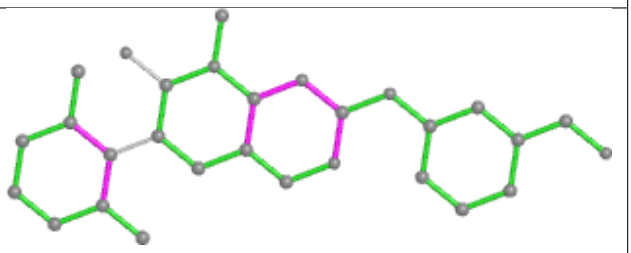
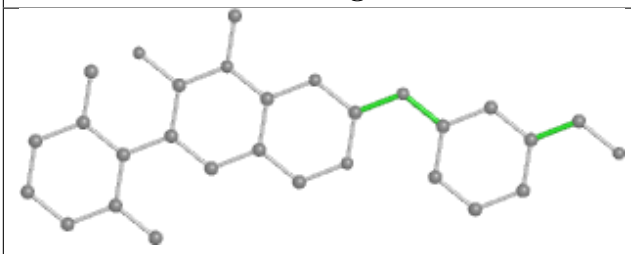
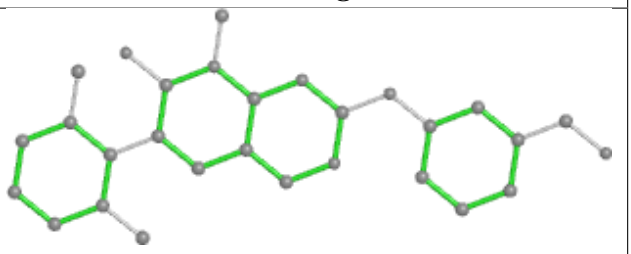
Mol	Chain	Res	Type	Atoms
2	A	538	MYR	C10-C11-C12-C13
2	A	538	MYR	C2-C3-C4-C5
2	A	538	MYR	C3-C4-C5-C6
2	A	538	MYR	C4-C5-C6-C7
2	A	538	MYR	C11-C12-C13-C14

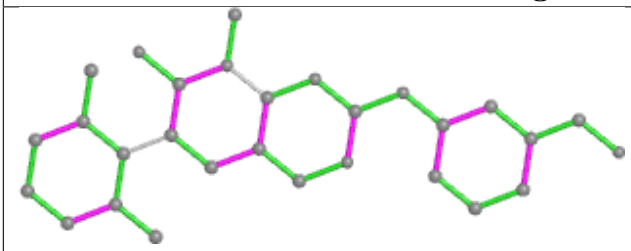
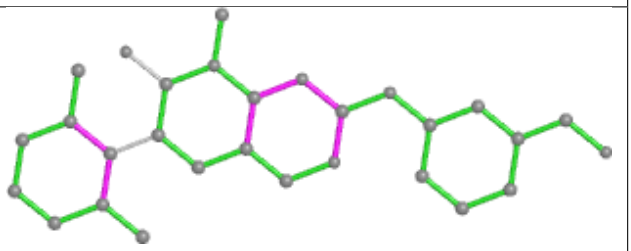
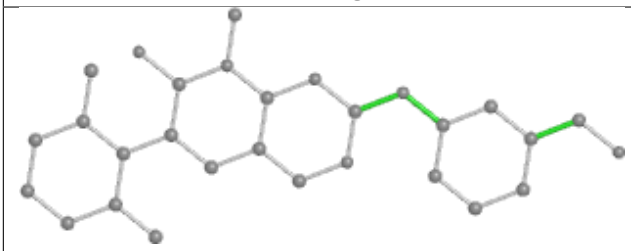
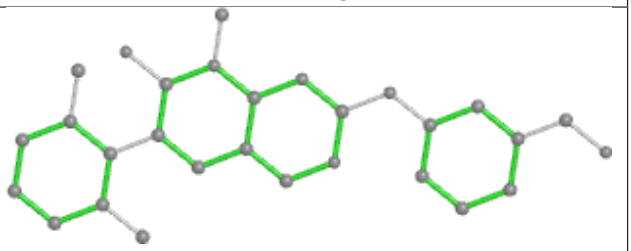
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	539	P16	1	0
3	B	538	P16	3	0
2	A	538	MYR	3	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 P16 A 539	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand P16 B 538	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	451/537 (83%)	0.76	21 (4%)	31	32	36, 73, 158, 221	0
1	B	365/537 (67%)	2.08	160 (43%)	0	0	161, 161, 198, 198	0
All	All	816/1074 (75%)	1.35	181 (22%)	0	1	36, 140, 198, 221	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	ASP	15.5
1	B	398	VAL	11.4
1	B	388	CYS	11.0
1	B	214	LEU	10.3
1	B	291	THR	9.1
1	B	212	ASN	8.7
1	B	399	ALA	8.4
1	B	277	GLU	8.1
1	B	205	VAL	7.9
1	B	490	LEU	7.1
1	B	342	LEU	6.9
1	B	218	VAL	6.8
1	B	151	VAL	6.5
1	B	217	LEU	6.5
1	B	163	GLY	6.0
1	B	203	LEU	6.0
1	B	267	LEU	5.9
1	B	389	LEU	5.8
1	B	394	HIS	5.4
1	A	295	ASP	5.3
1	B	261	ILE	5.2
1	B	204	TYR	5.1
1	B	345	TYR	5.1
1	B	164	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	351	ARG	5.0
1	B	280	TRP	5.0
1	B	459	TYR	5.0
1	B	180	ARG	4.9
1	B	318	VAL	4.9
1	B	408	THR	4.8
1	B	196	ASN	4.8
1	B	306	ALA	4.8
1	B	211	PHE	4.7
1	B	195	ILE	4.6
1	B	148	HIS	4.6
1	B	268	GLY	4.6
1	B	185	ARG	4.5
1	B	179	GLN	4.5
1	B	275	VAL	4.5
1	B	416	ALA	4.5
1	B	193	TYR	4.3
1	B	188	GLY	4.3
1	B	403	LEU	4.2
1	B	194	ARG	4.2
1	B	201	GLY	4.2
1	B	141	LEU	4.2
1	B	197	THR	4.1
1	B	462	ILE	4.1
1	B	302	PHE	4.1
1	A	408	THR	4.0
1	B	456	MET	4.0
1	B	285	LEU	4.0
1	B	357	VAL	3.9
1	B	184	LEU	3.9
1	B	343	LEU	3.9
1	A	291	THR	3.9
1	A	297	MET	3.8
1	B	150	PRO	3.8
1	B	221	HIS	3.8
1	B	229	ILE	3.8
1	B	330	PHE	3.8
1	B	202	LYS	3.8
1	B	168	PHE	3.7
1	B	175	SER	3.7
1	B	230	THR	3.7
1	B	283	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	383	LEU	3.6
1	B	381	ARG	3.6
1	B	227	GLY	3.6
1	B	451	ILE	3.6
1	B	309	MET	3.6
1	B	286	THR	3.6
1	A	278	GLY	3.5
1	B	323	VAL	3.5
1	B	317	LEU	3.5
1	B	390	VAL	3.5
1	B	444	PHE	3.5
1	B	454	TYR	3.5
1	A	296	THR	3.5
1	B	485	GLU	3.4
1	B	160	LEU	3.4
1	B	170	VAL	3.4
1	B	178	GLY	3.4
1	B	385	ALA	3.3
1	A	330	PHE	3.3
1	B	198	ALA	3.3
1	B	278	GLY	3.3
1	B	213	THR	3.3
1	B	325	THR	3.3
1	B	182	ILE	3.2
1	B	262	THR	3.2
1	B	169	LEU	3.2
1	B	146	TRP	3.2
1	B	448	LEU	3.1
1	B	418	ALA	3.1
1	B	387	ASN	3.1
1	B	331	TYR	3.1
1	B	142	GLU	3.1
1	B	407	MET	3.1
1	B	422	ILE	3.0
1	B	232	LEU	3.0
1	B	312	ILE	3.0
1	B	363	ALA	3.0
1	B	420	PHE	2.9
1	B	503	PRO	2.9
1	B	274	GLU	2.9
1	B	468	TYR	2.9
1	B	176	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	458	PRO	2.8
1	B	515	MET	2.8
1	B	452	ALA	2.8
1	B	171	ARG	2.8
1	B	423	LYS	2.8
1	B	477	MET	2.8
1	A	331	TYR	2.8
1	B	419	LYS	2.8
1	B	510	GLN	2.8
1	B	228	LEU	2.8
1	B	332	ILE	2.8
1	B	384	ALA	2.8
1	B	162	SER	2.7
1	B	396	VAL	2.7
1	B	159	LEU	2.6
1	A	409	GLY	2.6
1	B	290	LYS	2.6
1	B	424	TRP	2.6
1	B	174	GLU	2.6
1	A	292	LEU	2.5
1	B	372	TYR	2.5
1	B	346	LEU	2.5
1	B	287	VAL	2.5
1	A	230	THR	2.5
1	B	321	LEU	2.5
1	B	200	ASP	2.5
1	B	349	CYS	2.5
1	B	506	ALA	2.5
1	B	295	ASP	2.5
1	B	476	ARG	2.5
1	B	167	SER	2.4
1	B	256	MET	2.4
1	B	145	SER	2.4
1	A	256	MET	2.4
1	A	333	ILE	2.4
1	B	322	GLY	2.4
1	B	181	SER	2.3
1	B	209	SER	2.3
1	B	464	LEU	2.3
1	B	263	MET	2.3
1	B	517	GLN	2.3
1	B	206	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	397	LYS	2.3
1	B	405	ARG	2.3
1	B	356	ALA	2.3
1	A	332	ILE	2.3
1	B	199	SER	2.3
1	B	427	PRO	2.2
1	B	253	LYS	2.2
1	B	379	ILE	2.2
1	A	320	LEU	2.2
1	A	243	THR	2.2
1	B	225	ALA	2.2
1	B	226	ASP	2.2
1	A	254	TRP	2.2
1	B	336	PHE	2.2
1	B	478	GLU	2.1
1	B	269	GLY	2.1
1	B	183	SER	2.1
1	B	337	MET	2.1
1	B	393	ASN	2.1
1	A	319	GLN	2.1
1	B	409	GLY	2.1
1	B	401	PHE	2.1
1	B	339	TYR	2.1
1	A	298	GLU	2.1
1	B	305	GLU	2.1
1	B	449	TRP	2.0
1	A	277	GLU	2.0
1	A	203	LEU	2.0
1	B	480	PRO	2.0
1	B	497	TRP	2.0
1	B	505	PHE	2.0

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)

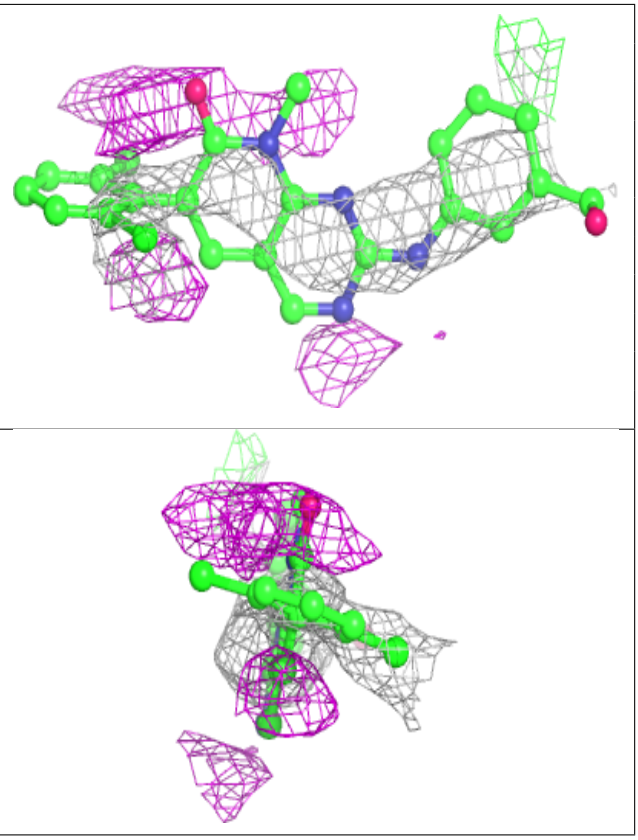
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P16	B	538	29/29	0.55	1.08	152,152,152,152	0
2	MYR	A	538	15/16	0.65	1.06	81,83,87,87	0
3	P16	A	539	29/29	0.86	0.52	82,84,89,97	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.

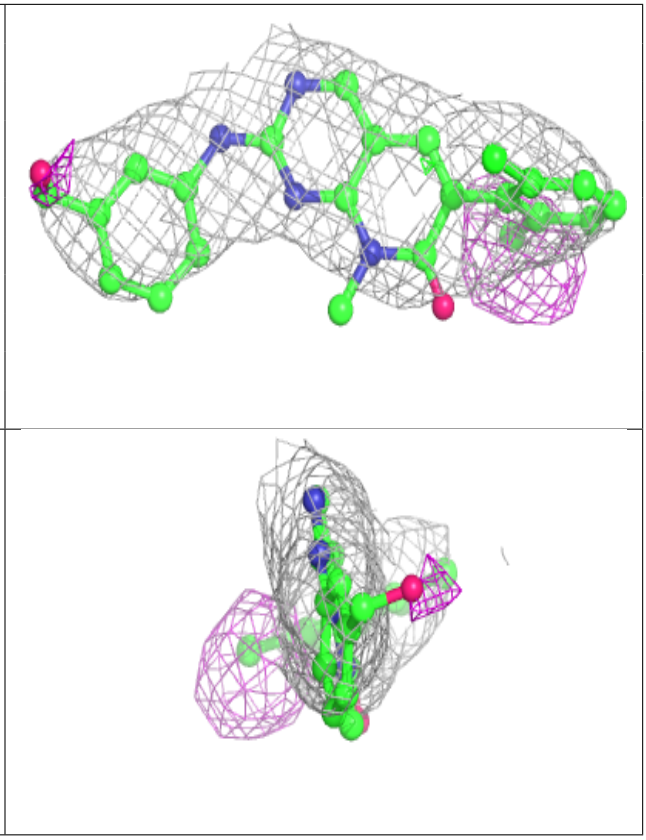
Electron density around P16 B 538:

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 P16 A 539:

$2mF_o$-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.