



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:54 PM UTC

PDB ID : 1OPL / pdb_00001opl
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

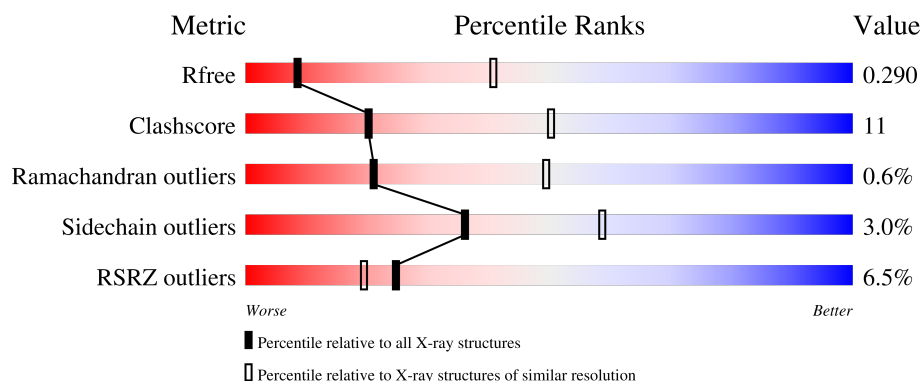
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	537	69% 13% • 16%
1	B	537	9% 50% 15% • 32%

2 Entry composition

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.

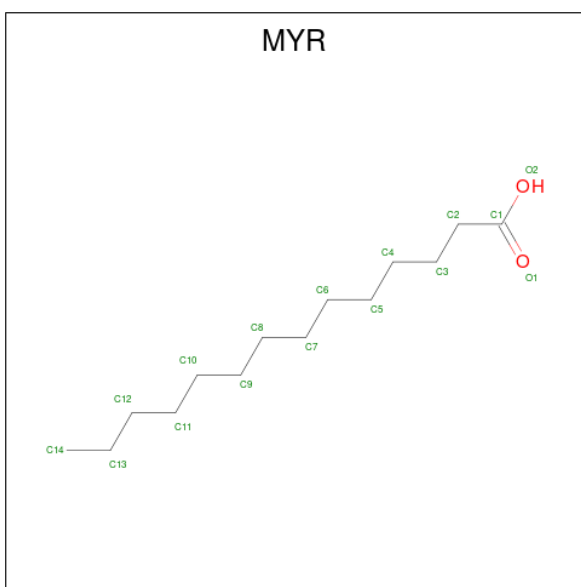
- Molecule 1 is a protein called proto-oncogene tyrosine-protein kinase.

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

There are 18 discrepancies between the modelled and reference sequences:

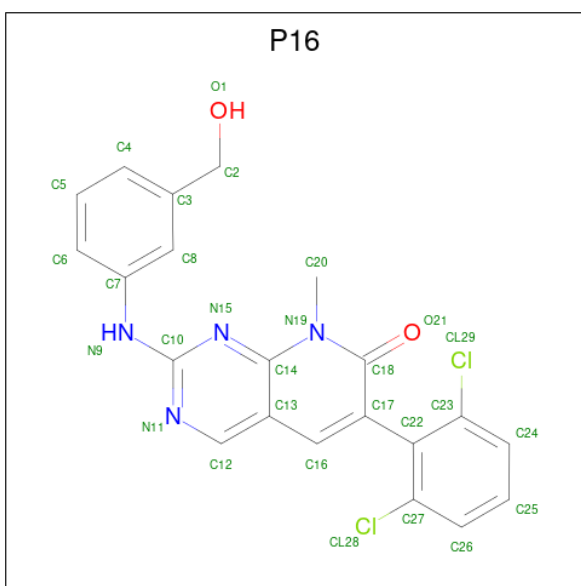
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ARG	LYS	engineered mutation	UNP P00519
A	30	ASP	GLU	engineered mutation	UNP P00519
A	382	ASN	ASP	engineered mutation	UNP P00519
A	532	GLU	-	cloning artifact	UNP P00519
A	533	ASN	-	cloning artifact	UNP P00519
A	534	LEU	-	cloning artifact	UNP P00519
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 (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



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

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



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

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.

- Chain A:
-
- 69% 13% 16%
- | Residue | Color | Percentage |
|---------|--------|------------|
| Y204 | Yellow | 13% |
| V205 | Yellow | 13% |
| R210 | Yellow | 13% |
| L214 | Yellow | 13% |
| T231 | Green | 69% |
| L232 | Green | 69% |
| H233 | Green | 69% |
| Y234 | Orange | 16% |
| P236 | Green | 69% |
| A236 | Green | 69% |
| T243 | Green | 69% |
| Y251 | Yellow | 13% |
| D252 | Orange | 16% |
| E255 | Green | 69% |
| M256 | Green | 69% |
| E257 | Green | 69% |
| R258 | Green | 69% |
| I261 | Yellow | 13% |
| G268 | Yellow | 13% |
| Q271 | Yellow | 13% |
| E277 | Yellow | 13% |
| W280 | Yellow | 13% |
| K281 | Yellow | 13% |
| K282 | Orange | 16% |
| Y283 | Orange | 16% |
| S284 | Green | 69% |
| L285 | Yellow | 13% |
| T291 | Green | 69% |
| E298 | Yellow | 13% |
| V299 | Yellow | 13% |
| E300 | Yellow | 13% |
| E301 | Yellow | 13% |
| G324 | Yellow | 13% |
| T325 | Yellow | 13% |
| R326 | Orange | 16% |
| E327 | Orange | 16% |
| Y331 | Yellow | 13% |
| I332 | Yellow | 13% |
| T338 | Yellow | 13% |
| Y339 | Yellow | 13% |
| N350 | Yellow | 13% |
| R351 | Green | 69% |
| D352 | Orange | 16% |

- Chain B:
-
- 9% 50% 15% 32%
- | Amino Acid | Count |
|------------|-------|
| ALA | 1 |
| ARG | 1 |
| ASN | 1 |
| ASP | 1 |
| CYS | 1 |
| GLN | 1 |
| GLY | 1 |
| ILE | 1 |
| LEU | 1 |
| LYS | 1 |
| PRO | 1 |
| PHE | 1 |
| THR | 1 |
| TRP | 1 |
| TYR | 1 |
| VAL | 1 |
| V151 | 1 |
| V155 | 1 |
| V156 | 1 |
| V160 | 1 |
| V161 | 1 |
| V162 | 1 |
| V163 | 1 |
| V175 | 1 |
| V176 | 1 |
| V177 | 1 |
| V182 | 1 |
| V185 | 1 |
| V190 | 1 |
| V194 | 1 |
| V203 | 1 |
| V204 | 1 |
| V205 | 1 |
| V210 | 1 |
| V214 | 1 |
| V215 | 1 |
| V218 | 1 |
| V231 | 1 |
| V232 | 1 |
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| V236 | 1 |
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| V252 | 1 |
| V253 | 1 |
| V254 | 1 |
| V255 | 1 |
| V256 | 1 |
| V257 | 1 |
| V258 | 1 |
| V259 | 1 |
| V260 | 1 |
| V261 | 1 |
| V267 | 1 |
| V268 | 1 |
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| V565 | 1 |
| V566 | 1 |
| V567 | 1 |
| V568 | 1 |
| V569 | 1 |
| V570 | 1 |
| V571 | 1 |
| V572 | 1 |
| V573 | |

GLU
LEU
GLY
LYS
GLU
ASN
LEU
TYR
PHE
GLN

4 Data and refinement statistics

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 29.95 – 3.42	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.95-3.42) 89.0 (29.95-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 3.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.306 , 0.315 0.276 , 0.290	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)	0.33 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.59	4/3723 (0.1%)	0.99	18/5049 (0.4%)
1	B	0.70	5/3031 (0.2%)	1.07	23/4105 (0.6%)
All	All	0.64	9/6754 (0.1%)	1.03	41/9154 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	LYS	N-CA	7.33	1.55	1.46
1	B	462	ILE	N-CA	6.51	1.54	1.46
1	B	459	TYR	N-CA	6.09	1.51	1.46
1	A	233	HIS	C-N	6.02	1.39	1.33
1	A	234	TYR	N-CA	5.69	1.52	1.46
1	B	398	VAL	CA-C	-5.48	1.46	1.52
1	A	460	PRO	N-CD	5.36	1.55	1.47
1	A	459	TYR	CA-C	5.29	1.59	1.52
1	B	295	ASP	N-CA	-5.23	1.39	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	VAL	N-CA-C	-11.48	100.77	111.67
1	A	205	VAL	N-CA-C	-11.41	100.83	111.67
1	B	466	GLN	OE1-CD-NE2	-9.80	112.80	122.60
1	A	463	ASP	CA-CB-CG	-9.80	102.80	112.60
1	B	510	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	A	338	THR	N-CA-C	8.55	121.54	111.71
1	B	338	THR	N-CA-C	8.55	121.54	111.71
1	A	515	MET	N-CA-C	7.36	121.50	112.23
1	B	295	ASP	CA-CB-CG	-7.13	105.47	112.60
1	B	459	TYR	CB-CA-C	-7.05	104.08	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	GLN	CG-CD-NE2	6.98	126.87	116.40
1	B	466	GLN	CG-CD-NE2	6.65	126.38	116.40
1	A	95	GLY	N-CA-C	-6.51	97.75	113.18
1	A	462	ILE	CA-C-N	-6.29	110.94	121.39
1	A	462	ILE	C-N-CA	-6.29	110.94	121.39
1	B	401	PHE	N-CA-C	-6.06	102.37	110.55
1	A	401	PHE	N-CA-C	-6.00	102.45	110.55
1	A	96	ASP	N-CA-C	5.99	119.42	111.75
1	B	464	LEU	CB-CA-C	5.85	123.28	110.18
1	A	114	HIS	N-CA-C	5.84	118.43	111.71
1	B	332	ILE	N-CA-C	-5.83	99.15	107.77
1	A	332	ILE	N-CA-C	-5.79	99.20	107.77
1	B	467	VAL	N-CA-C	5.70	115.90	110.42
1	A	83	ASN	CA-CB-CG	5.60	118.20	112.60
1	B	397	LYS	CA-C-N	5.54	129.31	121.66
1	B	397	LYS	C-N-CA	5.54	129.31	121.66
1	A	277	GLU	N-CA-C	-5.54	101.45	110.20
1	B	294	GLU	CA-C-N	-5.54	115.18	122.99
1	B	294	GLU	C-N-CA	-5.54	115.18	122.99
1	B	277	GLU	N-CA-C	-5.48	101.54	110.20
1	A	339	TYR	N-CA-C	5.44	119.90	113.16
1	A	467	VAL	N-CA-C	5.32	115.94	110.36
1	B	233	HIS	CA-C-N	-5.15	114.59	122.42
1	B	233	HIS	C-N-CA	-5.15	114.59	122.42
1	A	421	PRO	N-CA-C	-5.13	101.90	112.47
1	B	421	PRO	N-CA-C	-5.11	101.95	112.47
1	A	134	TYR	N-CA-C	-5.09	107.07	113.28
1	B	234	TYR	N-CA-CB	-5.06	100.76	110.17
1	B	465	SER	N-CA-C	5.02	117.65	111.82
1	B	439	SER	N-CA-C	-5.00	105.92	112.23
1	A	439	SER	N-CA-C	-5.00	105.93	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	0	3525	55	0
1	B	2954	0	2875	95	0
2	A	15	0	27	3	0
3	A	29	0	16	1	0
3	B	29	0	16	4	0
All	All	6655	0	6459	148	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 11.

All (148) 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:509:HIS:C	1:B:511:ALA:N	2.59	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:LEU:HD21	1:B:515:MET:C	2.28	0.59
1:B:364:THR:HG23	1:B:512:PHE:HB3	1.85	0.59
1:B:316:ASN:O	1:B:397:LYS:HA	2.03	0.58
1:B:258:ARG:C	1:B:260:ASP:H	2.10	0.57
1:B:295:ASP:OD1	1:B:295:ASP:C	2.45	0.57
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: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:A:529:LEU:HD11	2:A:538:MYR:C4	2.33	0.54
1:A:139:ASN:CG	1:A:139:ASN:O	2.51	0.53
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: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:296:THR:O	1:B:297:MET:C	2.53	0.52
1:B:326:ARG:C	1:B:327:GLU:HG3	2.35	0.51
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:463:ASP:C	1:A:465:SER:H	2.19	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:C	1:A:327:GLU:HG3	2.39	0.47
3:A:539:P16:H6	3:A:539:P16:N15	2.30	0.47
1:A:256:MET:HE1	1:A:261:ILE:HG12	1.98	0.46
1:B:255:GLU:HG3	1:B:326:ARG:NH2	2.31	0.46
1:B:160:LEU:HA	1:B:160:LEU:HD23	1.64	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:256:MET:HE1	1:B:261:ILE:HG12	1.97	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:473:LYS:HB3	1:B:473:LYS:HD3	1.97	0.45
1:A:251:TYR:O	1:A:252:ASP:C	2.59	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:B:463:ASP:C	1:B:465:SER:N	2.74	0.44
1:A:529:LEU:O	1:A:530:GLY:C	2.60	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:A:401:PHE:C	1:A:401:PHE:CD1	2.96	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:283:TYR:C	1:B:285:LEU:N	2.73	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:A:283:TYR:C	1:A:285:LEU:N	2.73	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:401:PHE:CD1	1:B:401:PHE:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:C	1:B:162:SER:N	2.76	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:A:252:ASP:C	1:A:252:ASP:OD1	2.63	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
1:A:256:MET:SD	1:A:324:CYS:SG	3.18	0.41
1:B:326:ARG:C	1:B:327:GLU:CG	2.92	0.41
1:B:509:HIS:C	1:B:511:ALA:H	2.27	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:A:425:THR:CG2	1:A:429:SER:HB2	2.51	0.41
1:B:258:ARG:C	1:B:260:ASP:N	2.77	0.41
1:B:463:ASP:C	1:B:465:SER:H	2.29	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:B:509:HIS:O	1:B:510:GLN:C	2.63	0.41
1:A:252:ASP:O	1:A:252:ASP:CG	2.64	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:B:272:TYR:CG	3:B:538:P16:H201	2.56	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:154:ASN:CG	1:A:360:LEU:HD21	2.46	0.40
1:A:194:ARG:HB2	1:A:194:ARG:HH11	1.87	0.40
1:A:256:MET:HE2	1:A:256:MET:HB2	1.97	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/537 (84%)	430 (96%)	17 (4%)	2 (0%)	30	59
1	B	361/537 (67%)	337 (93%)	21 (6%)	3 (1%)	16	44
All	All	810/1074 (75%)	767 (95%)	38 (5%)	5 (1%)	21	49

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

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%)	382 (97%)	11 (3%)	38	59
1	B	318/463 (69%)	308 (97%)	10 (3%)	35	58
All	All	711/926 (77%)	690 (97%)	21 (3%)	36	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LEU

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Mol	Chain	Res	Type
1	A	139	ASN
1	A	203	LEU
1	A	214	LEU
1	A	231	THR
1	A	233	HIS
1	A	283	TYR
1	A	298	GLU
1	A	327	GLU
1	A	448	LEU
1	A	490	LEU
1	B	203	LEU
1	B	214	LEU
1	B	231	THR
1	B	258	ARG
1	B	260	ASP
1	B	283	TYR
1	B	297	MET
1	B	327	GLU
1	B	448	LEU
1	B	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	144	HIS
1	A	233	HIS
1	A	240	ASN
1	A	350	ASN
1	A	393	ASN
1	B	144	HIS
1	B	319	GLN
1	B	350	ASN
1	B	509	HIS
1	B	517	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	-	32,32,32	1.97	13 (40%)	43,46,46	1.12	4 (9%)
3	P16	B	538	-	32,32,32	1.96	13 (40%)	43,46,46	1.12	4 (9%)
2	MYR	A	538	-	13,14,15	0.56	0	12,13,15	0.49	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	-	-	2/10/10/10	0/4/4/4
3	P16	B	538	-	-	2/10/10/10	0/4/4/4
2	MYR	A	538	-	-	5/12/12/13	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	538	P16	C18-N19	4.50	1.44	1.38
3	A	539	P16	C18-N19	4.47	1.44	1.38
3	A	539	P16	C17-C18	3.22	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	538	P16	C17-C18	3.15	1.51	1.46
3	B	538	P16	C10-N11	3.03	1.38	1.34
3	A	539	P16	C10-N11	3.02	1.38	1.34
3	A	539	P16	C22-C23	3.02	1.44	1.39
3	B	538	P16	C22-C23	2.95	1.44	1.39
3	B	538	P16	C8-C7	2.81	1.44	1.39
3	B	538	P16	C4-C3	2.79	1.44	1.38
3	A	539	P16	C4-C3	2.76	1.44	1.38
3	A	539	P16	C6-C7	2.75	1.43	1.39
3	A	539	P16	C8-C7	2.73	1.43	1.39
3	B	538	P16	C6-C7	2.73	1.43	1.39
3	A	539	P16	C5-C6	2.56	1.43	1.38
3	A	539	P16	C26-C27	2.48	1.43	1.38
3	B	538	P16	C5-C6	2.46	1.43	1.38
3	B	538	P16	C26-C27	2.45	1.43	1.38
3	A	539	P16	C25-C24	2.39	1.43	1.38
3	B	538	P16	C25-C24	2.38	1.43	1.38
3	B	538	P16	C25-C26	2.36	1.42	1.38
3	A	539	P16	C25-C26	2.36	1.42	1.38
3	A	539	P16	C24-C23	2.23	1.43	1.38
3	B	538	P16	C24-C23	2.21	1.43	1.38
3	B	538	P16	C22-C27	2.07	1.42	1.39
3	A	539	P16	C22-C27	2.03	1.42	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	538	P16	C22-C17-C18	-2.64	116.82	119.36
3	A	539	P16	C22-C17-C18	-2.60	116.86	119.36
3	A	539	P16	C20-N19-C18	2.58	119.83	117.34
3	B	538	P16	C20-N19-C18	2.57	119.82	117.34
3	B	538	P16	O21-C18-N19	-2.48	117.65	121.22
3	A	539	P16	O21-C18-N19	-2.45	117.69	121.22
3	B	538	P16	N11-C10-N15	-2.14	124.35	126.42
3	A	539	P16	N11-C10-N15	-2.11	124.38	126.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

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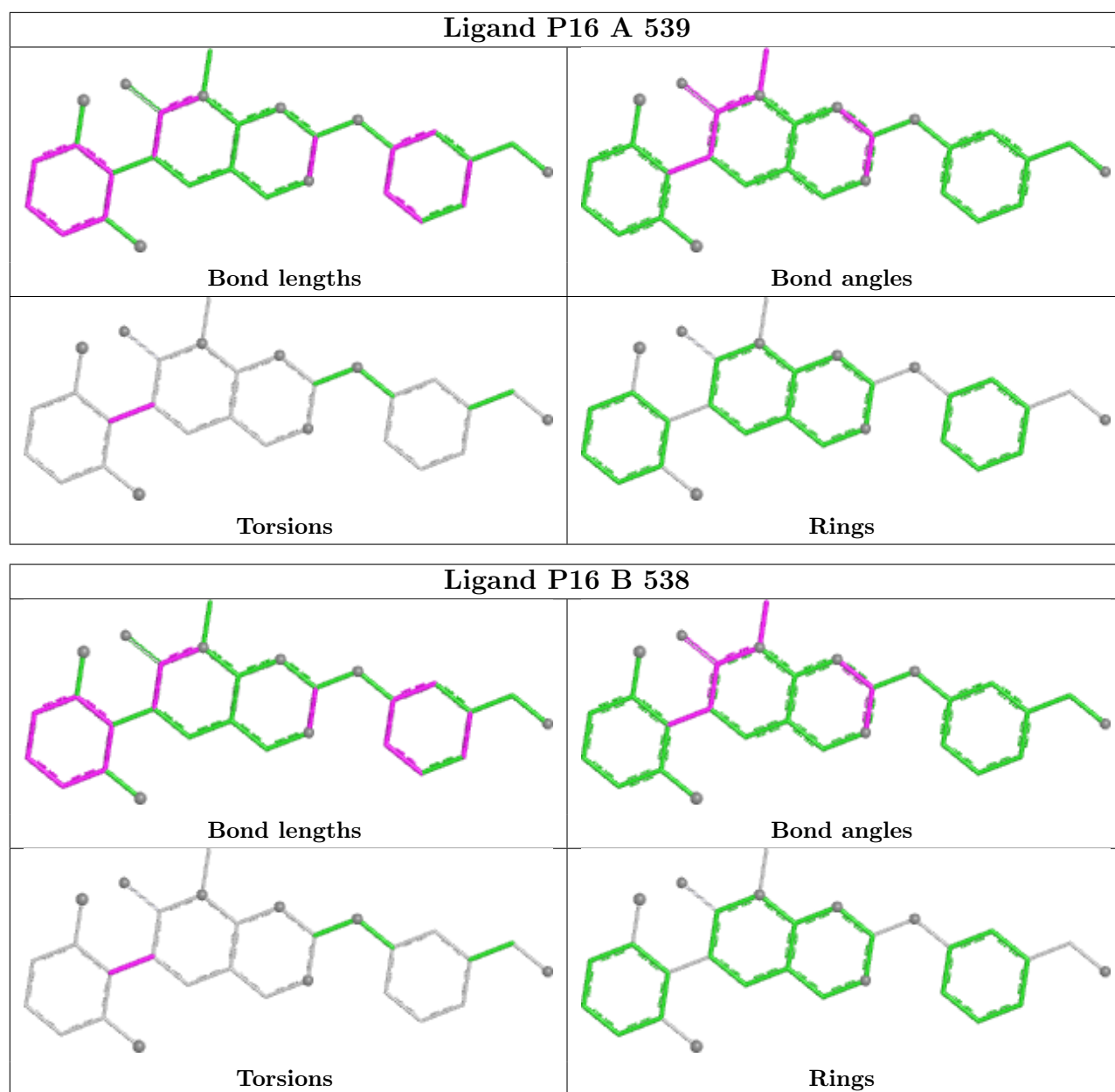
Mol	Chain	Res	Type	Atoms
2	A	538	MYR	C3-C4-C5-C6
3	A	539	P16	C18-C17-C22-C27
3	B	538	P16	C18-C17-C22-C27
2	A	538	MYR	C4-C5-C6-C7
3	A	539	P16	C18-C17-C22-C23
3	B	538	P16	C18-C17-C22-C23
2	A	538	MYR	C11-C12-C13-C14

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	539	P16	1	0
3	B	538	P16	4	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	451/537 (83%)	-0.01	5 (1%) 78 65	36, 73, 158, 221	0
1	B	365/537 (67%)	0.92	48 (13%) 7 8	161, 161, 198, 198	0
All	All	816/1074 (75%)	0.41	53 (6%) 25 19	36, 140, 198, 221	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	398	VAL	8.4
1	B	388	CYS	7.5
1	B	400	ASP	7.0
1	B	342	LEU	5.6
1	B	451	ILE	3.9
1	B	467	VAL	3.9
1	B	459	TYR	3.8
1	B	462	ILE	3.8
1	B	383	LEU	3.4
1	B	422	ILE	3.4
1	B	458	PRO	3.4
1	B	214	LEU	3.3
1	B	283	TYR	3.3
1	B	291	THR	3.3
1	B	280	TRP	3.2
1	B	387	ASN	2.9
1	B	470	LEU	2.9
1	B	390	VAL	2.9
1	B	321	LEU	2.8
1	B	345	TYR	2.7
1	A	299	VAL	2.7
1	B	356	ALA	2.7
1	B	277	GLU	2.6
1	B	363	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	399	ALA	2.6
1	B	343	LEU	2.6
1	B	403	LEU	2.5
1	B	424	TRP	2.5
1	A	243	THR	2.5
1	B	444	PHE	2.5
1	B	475	TYR	2.5
1	B	491	MET	2.4
1	B	182	ILE	2.4
1	B	430	LEU	2.3
1	B	358	VAL	2.3
1	B	456	MET	2.3
1	B	318	VAL	2.3
1	B	215	ALA	2.3
1	A	430	LEU	2.2
1	B	329	PRO	2.2
1	B	267	LEU	2.2
1	A	291	THR	2.2
1	B	362	MET	2.2
1	A	331	TYR	2.1
1	B	490	LEU	2.1
1	B	218	VAL	2.1
1	B	366	ILE	2.1
1	B	454	TYR	2.1
1	B	466	GLN	2.1
1	B	503	PRO	2.1
1	B	447	LEU	2.1
1	B	463	ASP	2.1
1	B	317	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

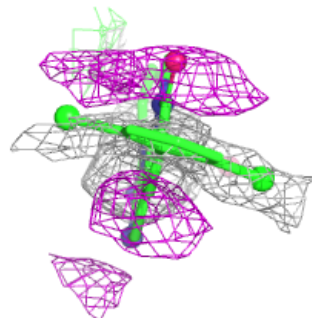
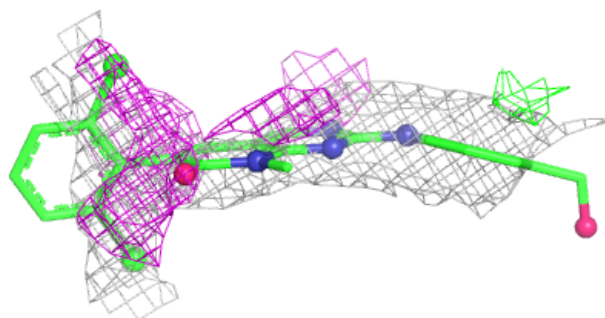
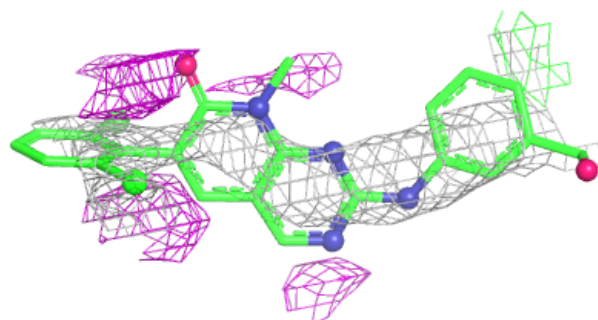
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.58	0.20	152,152,152,152	0
3	P16	A	539	29/29	0.84	0.18	82,84,89,97	0
2	MYR	A	538	15/16	0.90	0.25	81,83,87,87	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.

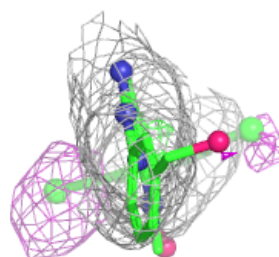
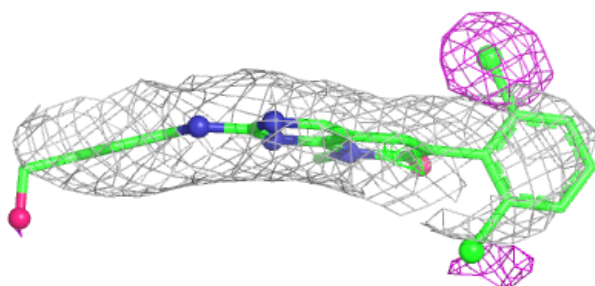
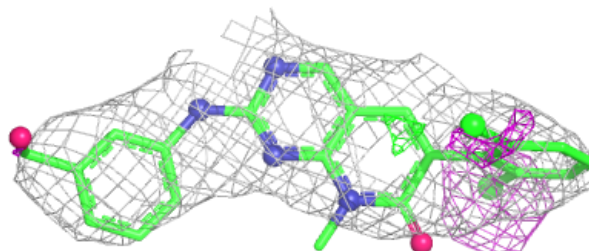
Electron density around P16 B 538:

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 ⓘ

There are no such residues in this entry.