



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:39 AM UTC

PDB ID : 3F3U / pdb_00003f3u
Title : Kinase domain of cSrc in complex with inhibitor RL37 (Type III)
Authors : Gruetter, C.; Klueter, S.; Getlik, M.; Rauh, D.
Deposited on : 2008-10-31
Resolution : 2.50 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 ⓘ 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

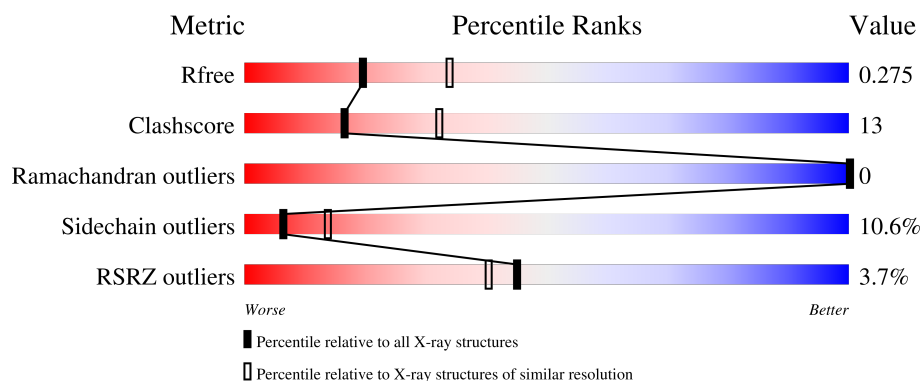
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	286	
1	B	286	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4355 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.

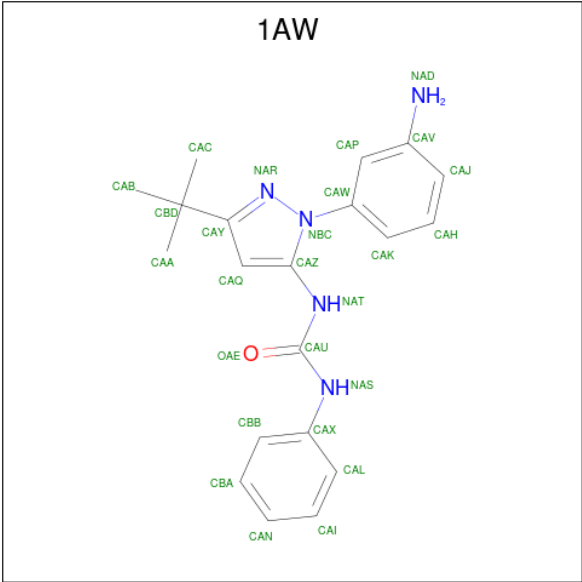
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2103	1351	350	384	18			
1	B	259	Total	C	N	O	S	0	0	0
			2088	1342	348	381	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
A	345	CYS	SER	engineered mutation	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523
B	345	CYS	SER	engineered mutation	UNP P00523

- Molecule 2 is 1-[1-(3-aminophenyl)-3-tert-butyl-1H-pyrazol-5-yl]-3-phenylurea (CCD ID: 1AW) (formula: C₂₀H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	20	5	1		
2	A	1	Total	C	N	O	0	0
			26	20	5	1		
2	B	1	Total	C	N	O	0	0
			26	20	5	1		

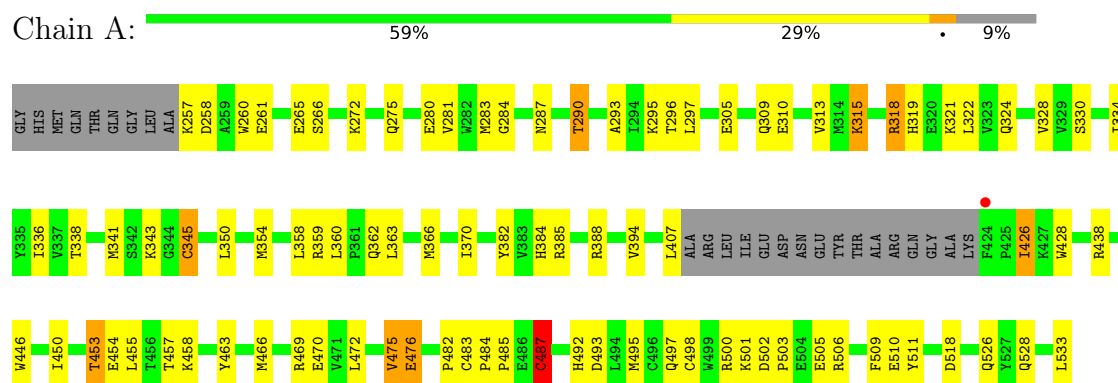
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	45	Total	O	0	0
			45	45		

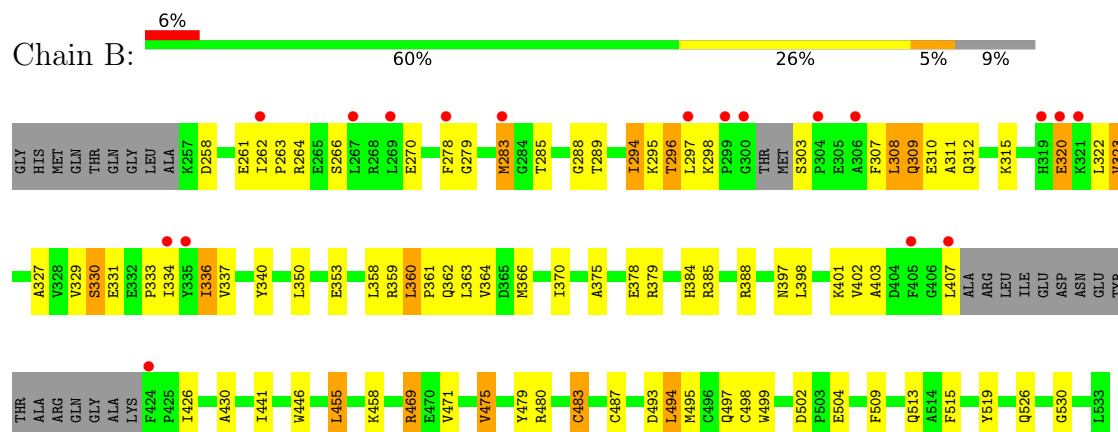
3 Residue-property plots

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 Src



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.09Å 63.53Å 73.99Å 78.94° 89.37° 90.06°	Depositor
Resolution (Å)	36.59 – 2.50 36.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.59-2.50) 97.3 (36.59-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.222 , 0.281 0.219 , 0.275	Depositor DCC
R_{free} test set	1014 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4355	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.49% 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: 1AW

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	0.97	2/2155 (0.1%)	1.14	7/2917 (0.2%)
1	B	0.96	1/2139 (0.0%)	1.11	7/2894 (0.2%)
All	All	0.96	3/4294 (0.1%)	1.13	14/5811 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	THR	CA-CB	7.75	1.64	1.53
1	A	475	VAL	CA-CB	5.22	1.62	1.54
1	B	479	TYR	CA-C	5.12	1.59	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	CYS	CA-C-N	7.35	127.95	120.38
1	B	483	CYS	C-N-CA	7.35	127.95	120.38
1	A	370	ILE	N-CA-C	-6.73	103.92	110.72
1	B	330	SER	N-CA-C	6.66	118.23	110.97
1	A	290	THR	N-CA-C	6.61	119.93	108.76
1	A	258	ASP	N-CA-C	6.44	118.45	109.31
1	A	457	THR	N-CA-C	-6.09	105.16	112.59
1	B	370	ILE	N-CA-C	-5.74	105.14	110.53
1	A	487	CYS	CA-C-N	5.74	125.75	119.90
1	A	487	CYS	C-N-CA	5.74	125.75	119.90
1	A	454	GLU	N-CA-C	-5.69	105.06	112.23
1	B	519	TYR	N-CA-C	5.57	118.07	111.33
1	B	303	SER	CA-C-N	5.12	126.24	119.84
1	B	303	SER	C-N-CA	5.12	126.24	119.84

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	2103	0	2089	50	0
1	B	2088	0	2072	57	0
2	A	52	0	46	7	0
2	B	26	0	23	3	0
3	A	41	0	0	3	0
3	B	45	0	0	3	0
All	All	4355	0	4230	110	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 13.

All (110) 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:345:CYS:SG	2:A:534:1AW:NAD	2.32	1.01
1:B:294:ILE:HG23	1:B:337:VAL:HG22	1.52	0.90
1:B:285:THR:HG22	1:B:288:GLY:HA2	1.57	0.86
1:A:363:LEU:HD13	1:A:455:LEU:O	1.77	0.85
1:B:263:PRO:HD2	1:B:266:SER:OG	1.83	0.79
1:B:359:ARG:H	1:B:362:GLN:HE21	1.33	0.76
1:B:469:ARG:HH11	1:B:469:ARG:CG	1.98	0.74
1:B:310:GLU:HG3	2:B:1:1AW:CAV	2.18	0.74
1:A:453:THR:HG23	3:A:18:HOH:O	1.87	0.74
1:B:493:ASP:O	1:B:497:GLN:HG3	1.88	0.74
1:B:469:ARG:HH11	1:B:469:ARG:HG2	1.53	0.73
1:B:285:THR:CG2	1:B:288:GLY:HA2	2.19	0.73
1:A:322:LEU:HD13	2:A:1:1AW:HAB	1.72	0.72
1:A:266:SER:HB2	1:A:287:ASN:HD22	1.58	0.69
1:B:298:LYS:HB3	1:B:333:PRO:HB3	1.73	0.68
1:B:526:GLN:HG2	3:B:8:HOH:O	1.94	0.68
1:A:500:ARG:HD3	1:A:505:GLU:HB3	1.76	0.67
1:B:494:LEU:HG	1:B:515:PHE:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG11	1:A:382:TYR:OH	1.94	0.67
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.31	0.65
1:B:359:ARG:H	1:B:362:GLN:NE2	1.94	0.64
1:A:476:GLU:HA	1:A:476:GLU:OE1	1.97	0.64
1:B:323:VAL:HG21	1:B:403:ALA:HB2	1.81	0.62
1:A:281:VAL:HG23	2:A:534:1AW:HABB	1.84	0.60
1:B:310:GLU:HG3	2:B:1:1AW:CAP	2.35	0.57
1:B:323:VAL:HG23	1:B:402:VAL:O	2.05	0.57
1:A:450:ILE:O	1:A:453:THR:HG22	2.06	0.56
1:A:426:ILE:HD11	1:A:472:LEU:HD21	1.87	0.56
1:B:283:MET:HE2	1:B:340:TYR:OH	2.08	0.54
1:A:518:ASP:OD2	3:A:85:HOH:O	2.18	0.54
1:A:280:GLU:H	1:A:296:THR:HB	1.72	0.54
1:A:260:TRP:CZ2	1:A:315:LYS:HG2	2.43	0.54
1:B:378:GLU:HB2	1:B:441:ILE:HG12	1.89	0.54
1:B:322:LEU:HD22	1:B:402:VAL:HB	1.90	0.53
1:B:363:LEU:HD13	1:B:455:LEU:O	2.09	0.53
1:B:430:ALA:HB2	1:B:446:TRP:CB	2.38	0.53
1:A:463:TYR:HA	3:A:48:HOH:O	2.08	0.52
1:B:320:GLU:O	1:B:401:LYS:HE2	2.10	0.52
1:A:319:HIS:CD2	1:A:321:LYS:H	2.28	0.52
1:A:266:SER:HB2	1:A:287:ASN:ND2	2.25	0.51
1:B:469:ARG:CG	1:B:469:ARG:NH1	2.64	0.51
1:B:261:GLU:OE1	1:B:330:SER:HB2	2.11	0.51
1:B:311:ALA:O	1:B:315:LYS:HG3	2.11	0.50
1:B:264:ARG:HE	1:B:329:VAL:HG11	1.76	0.50
1:B:279:GLY:HA3	1:B:296:THR:O	2.12	0.50
1:A:438:ARG:HH21	1:A:503:PRO:HG2	1.75	0.50
1:A:261:GLU:OE1	1:A:330:SER:HB2	2.11	0.49
1:B:307:PHE:HE2	1:B:334:ILE:CD1	2.25	0.49
1:B:309:GLN:HA	1:B:312:GLN:HG2	1.93	0.49
1:A:309:GLN:NE2	1:A:309:GLN:HA	2.27	0.49
1:A:384:HIS:O	1:A:385:ARG:HB2	2.12	0.49
1:B:397:ASN:O	1:B:398:LEU:HB2	2.11	0.49
1:B:359:ARG:HB2	1:B:362:GLN:HE22	1.78	0.49
1:B:310:GLU:OE1	1:B:336:ILE:HD12	2.13	0.49
2:B:1:1AW:NAT	2:B:1:1AW:HAP	2.28	0.49
1:A:341:MET:H	2:A:534:1AW:HAN	1.76	0.48
1:A:493:ASP:O	1:A:497:GLN:HG3	2.13	0.48
1:B:307:PHE:CE2	1:B:334:ILE:HD11	2.49	0.48
1:A:318:ARG:HB3	1:A:318:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:1AW:HAL	2:A:1:1AW:OAE	2.14	0.48
1:B:285:THR:HG22	1:B:288:GLY:CA	2.35	0.48
1:B:358:LEU:O	1:B:458:LYS:NZ	2.46	0.47
1:B:334:ILE:C	1:B:334:ILE:HD12	2.39	0.47
1:B:307:PHE:HE2	1:B:334:ILE:HD11	1.78	0.47
1:B:526:GLN:CG	3:B:8:HOH:O	2.57	0.47
1:A:483:CYS:SG	1:A:487:CYS:O	2.72	0.47
1:A:426:ILE:CD1	1:A:472:LEU:HD21	2.45	0.47
1:A:260:TRP:HE1	1:A:315:LYS:HD2	1.80	0.46
1:B:530:GLY:HA3	3:B:77:HOH:O	2.15	0.46
1:A:492:HIS:O	1:A:495:MET:HB2	2.16	0.46
1:A:319:HIS:HD2	1:A:321:LYS:H	1.63	0.46
1:A:426:ILE:O	1:A:426:ILE:HG13	2.15	0.46
1:A:283:MET:HG2	1:A:284:GLY:N	2.30	0.45
1:A:358:LEU:O	1:A:458:LYS:NZ	2.49	0.45
1:A:272:LYS:CE	1:A:275:GLN:HB3	2.47	0.45
1:A:295:LYS:HB3	1:A:336:ILE:HB	1.99	0.45
1:A:293:ALA:HB3	1:A:338:THR:OG1	2.16	0.45
1:B:471:VAL:O	1:B:475:VAL:HG13	2.17	0.44
1:B:362:GLN:O	1:B:366:MET:HG3	2.18	0.44
1:B:308:LEU:HD22	1:B:308:LEU:HA	1.80	0.44
1:B:295:LYS:HE2	1:B:307:PHE:HZ	1.82	0.43
1:B:480:ARG:NH2	1:B:499:TRP:O	2.50	0.43
1:A:482:PRO:O	1:A:484:PRO:HD3	2.18	0.43
1:A:343:LYS:HB2	1:A:394:VAL:O	2.18	0.43
1:B:262:ILE:HG12	1:B:327:ALA:HB1	2.00	0.43
1:A:358:LEU:O	1:A:359:ARG:NH1	2.40	0.43
1:B:384:HIS:O	1:B:385:ARG:HB2	2.19	0.43
2:A:534:1AW:OAE	2:A:534:1AW:HAL	2.18	0.43
1:B:359:ARG:O	1:B:360:LEU:C	2.61	0.43
1:A:446:TRP:C	1:A:446:TRP:CD1	2.96	0.42
1:A:466:MET:HA	1:A:470:GLU:OE1	2.19	0.42
1:A:485:PRO:O	1:A:533:LEU:HD12	2.19	0.42
1:B:495:MET:O	1:B:498:CYS:HB2	2.19	0.42
1:A:511:TYR:CD2	1:A:511:TYR:C	2.97	0.42
1:A:318:ARG:NH2	1:A:324:GLN:NE2	2.67	0.42
1:B:294:ILE:CG2	1:B:337:VAL:HG22	2.35	0.42
1:B:483:CYS:SG	1:B:487:CYS:O	2.78	0.42
1:B:509:PHE:O	1:B:513:GLN:N	2.45	0.41
1:A:310:GLU:HA	2:A:1:1AW:CAH	2.50	0.41
1:A:426:ILE:HD11	1:A:472:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ASP:HB3	1:A:505:GLU:OE1	2.19	0.41
1:B:375:ALA:O	1:B:379:ARG:HG3	2.21	0.41
1:A:498:CYS:O	1:A:506:ARG:HD3	2.19	0.41
1:A:509:PHE:O	1:A:510:GLU:C	2.62	0.41
1:B:360:LEU:O	1:B:361:PRO:C	2.63	0.41
1:A:362:GLN:O	1:A:366:MET:HG3	2.21	0.40
1:B:262:ILE:HD12	1:B:266:SER:HB2	2.04	0.40
1:B:360:LEU:HD22	1:B:364:VAL:HG23	2.04	0.40
1:B:502:ASP:OD1	1:B:502:ASP:C	2.65	0.40
1:B:378:GLU:HB2	1:B:441:ILE:CD1	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	257/286 (90%)	242 (94%)	15 (6%)	0	100	100
1	B	253/286 (88%)	235 (93%)	18 (7%)	0	100	100
All	All	510/572 (89%)	477 (94%)	33 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/245 (93%)	204 (90%)	23 (10%)	7	15
1	B	225/245 (92%)	200 (89%)	25 (11%)	6	12
All	All	452/490 (92%)	404 (89%)	48 (11%)	6	14

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	LYS
1	A	265	GLU
1	A	290	THR
1	A	297	LEU
1	A	305	GLU
1	A	315	LYS
1	A	318	ARG
1	A	328	VAL
1	A	334	ILE
1	A	345	CYS
1	A	350	LEU
1	A	354	MET
1	A	360	LEU
1	A	407	LEU
1	A	426	ILE
1	A	453	THR
1	A	469	ARG
1	A	475	VAL
1	A	476	GLU
1	A	487	CYS
1	A	501	LYS
1	A	526	GLN
1	A	528	GLN
1	B	258	ASP
1	B	270	GLU
1	B	278	PHE
1	B	283	MET
1	B	289	THR
1	B	294	ILE
1	B	296	THR
1	B	297	LEU
1	B	308	LEU
1	B	309	GLN
1	B	320	GLU
1	B	323	VAL

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Mol	Chain	Res	Type
1	B	331	GLU
1	B	336	ILE
1	B	350	LEU
1	B	353	GLU
1	B	360	LEU
1	B	388	ARG
1	B	407	LEU
1	B	426	ILE
1	B	455	LEU
1	B	469	ARG
1	B	475	VAL
1	B	494	LEU
1	B	504	GLU

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	287	ASN
1	A	309	GLN
1	A	319	HIS
1	A	324	GLN
1	A	397	ASN
1	A	468	ASN
1	A	492	HIS
1	B	275	GLN
1	B	324	GLN
1	B	362	GLN
1	B	528	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	1AW	B	1	-	28,28,28	2.30	7 (25%)	38,40,40	1.77	8 (21%)
2	1AW	A	1	-	28,28,28	2.28	8 (28%)	38,40,40	1.74	9 (23%)
2	1AW	A	534	-	28,28,28	2.11	6 (21%)	38,40,40	1.85	5 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1AW	B	1	-	-	0/18/18/18	0/3/3/3
2	1AW	A	1	-	-	0/18/18/18	0/3/3/3
2	1AW	A	534	-	-	4/18/18/18	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	1AW	NBC-NAR	-7.24	1.23	1.39
2	B	1	1AW	NBC-NAR	-7.15	1.23	1.39
2	A	534	1AW	NBC-NAR	-6.80	1.24	1.39
2	A	534	1AW	CAW-NBC	-4.93	1.34	1.43
2	B	1	1AW	CAW-NBC	-4.62	1.34	1.43
2	A	1	1AW	CAW-NBC	-4.61	1.34	1.43
2	B	1	1AW	CAQ-CAY	-4.19	1.33	1.39
2	A	1	1AW	CAX-NAS	-3.93	1.33	1.41
2	B	1	1AW	CAZ-NAT	-3.90	1.34	1.39
2	A	1	1AW	CAQ-CAY	-3.80	1.33	1.39
2	B	1	1AW	CAQ-CAZ	-3.66	1.32	1.37
2	A	534	1AW	CBD-CAY	3.48	1.58	1.52
2	B	1	1AW	CAZ-NBC	-3.15	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	1AW	CAQ-CAZ	-3.02	1.33	1.37
2	A	534	1AW	CAQ-CAY	-2.96	1.35	1.39
2	A	534	1AW	CAX-NAS	-2.92	1.35	1.41
2	A	1	1AW	CAZ-NBC	-2.68	1.34	1.36
2	A	1	1AW	CAZ-NAT	-2.63	1.35	1.39
2	B	1	1AW	CAU-NAT	-2.32	1.34	1.39
2	A	534	1AW	CAZ-NBC	-2.02	1.34	1.36
2	A	1	1AW	CAU-NAT	-2.01	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	534	1AW	CAW-NBC-CAZ	-6.40	123.50	129.78
2	A	1	1AW	CAY-NAR-NBC	4.88	108.36	104.27
2	A	534	1AW	CAW-NBC-NAR	4.65	125.42	118.67
2	B	1	1AW	CAY-NAR-NBC	4.47	108.02	104.27
2	B	1	1AW	CAQ-CAZ-NAT	-4.41	125.38	132.60
2	A	534	1AW	CAY-NAR-NBC	4.41	107.97	104.27
2	A	1	1AW	CAQ-CAZ-NAT	-3.95	126.15	132.60
2	A	1	1AW	NAT-CAZ-NBC	3.82	126.56	120.11
2	A	534	1AW	CBD-CAY-NAR	3.75	125.38	120.42
2	B	1	1AW	NAT-CAZ-NBC	3.68	126.32	120.11
2	B	1	1AW	CBD-CAY-NAR	3.48	125.02	120.42
2	A	1	1AW	CBD-CAY-NAR	3.17	124.61	120.42
2	B	1	1AW	CAW-NBC-NAR	3.00	123.02	118.67
2	A	534	1AW	CAQ-CAY-NAR	-2.77	108.59	111.86
2	A	1	1AW	CAP-CAW-NBC	2.71	123.20	119.27
2	B	1	1AW	CAW-NBC-CAZ	-2.63	127.20	129.78
2	A	1	1AW	CAW-NBC-NAR	2.45	122.23	118.67
2	A	1	1AW	CAW-NBC-CAZ	-2.38	127.45	129.78
2	B	1	1AW	CAZ-NBC-NAR	-2.35	109.78	111.82
2	B	1	1AW	CBD-CAY-CAQ	-2.25	125.47	128.66
2	A	1	1AW	CAQ-CAY-NAR	-2.23	109.23	111.86
2	A	1	1AW	CAB-CBD-CAY	-2.01	106.21	109.63

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	534	1AW	CAP-CAW-NBC-NAR
2	A	534	1AW	CAK-CAW-NBC-NAR
2	A	534	1AW	CAP-CAW-NBC-CAZ

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Mol	Chain	Res	Type	Atoms
2	A	534	1AW	CAK-CAW-NBC-CAZ

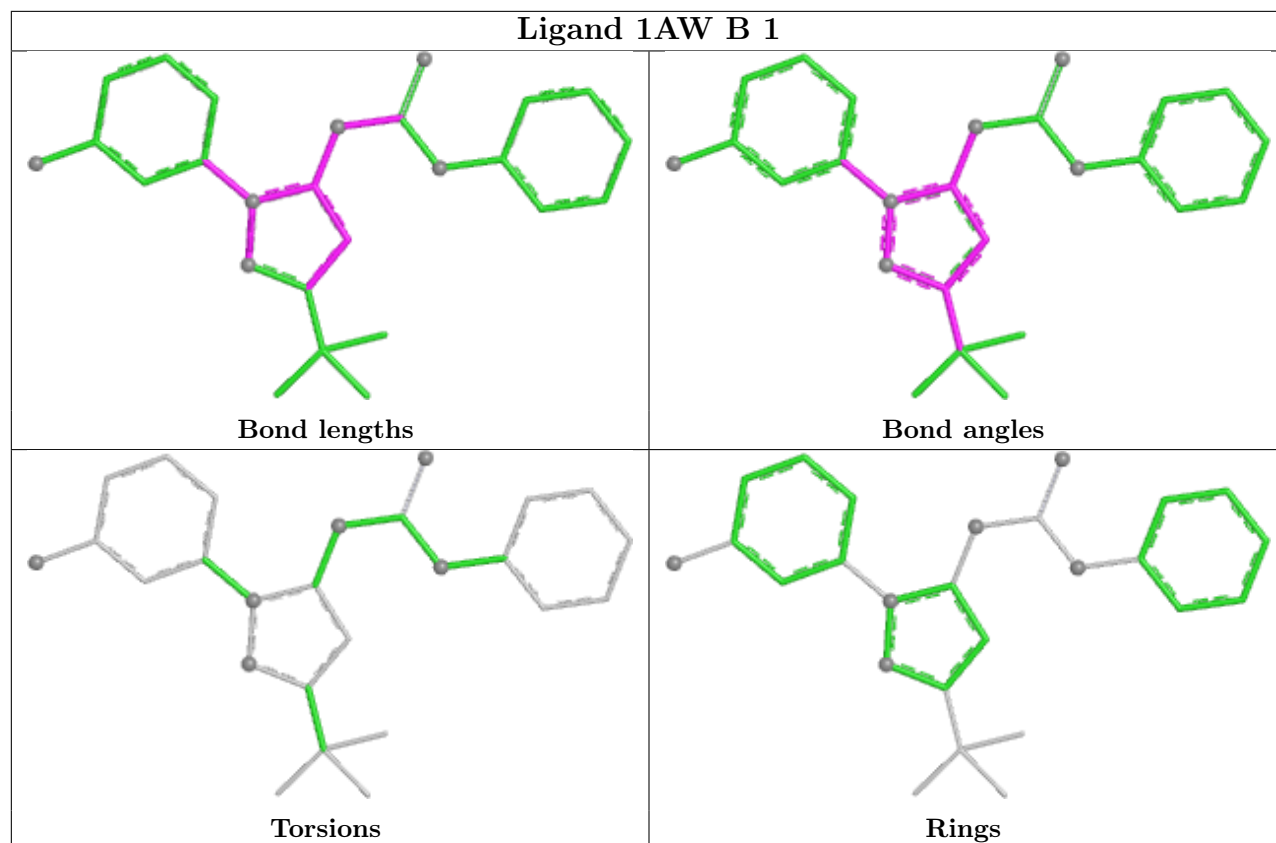
There are no ring outliers.

3 monomers are involved in 10 short contacts:

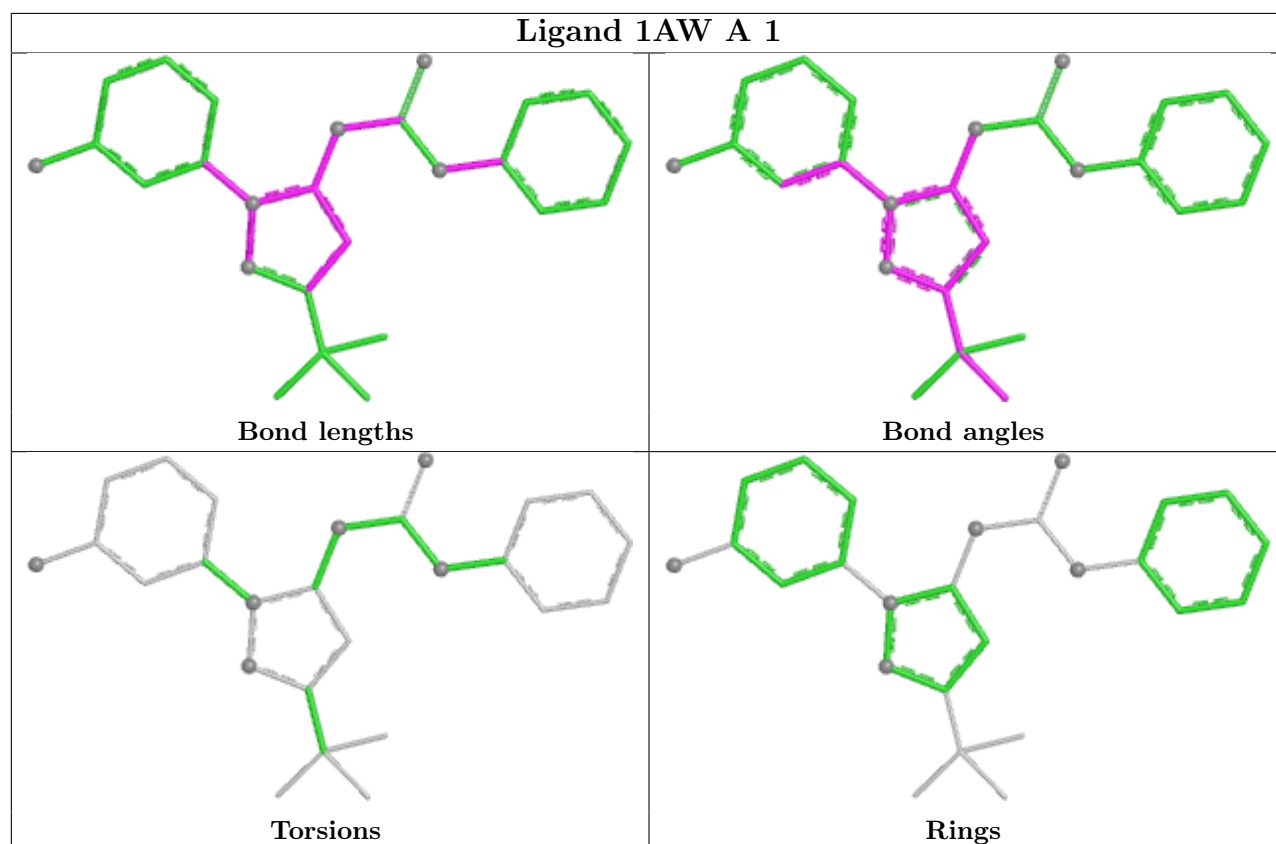
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	1AW	3	0
2	A	1	1AW	3	0
2	A	534	1AW	4	0

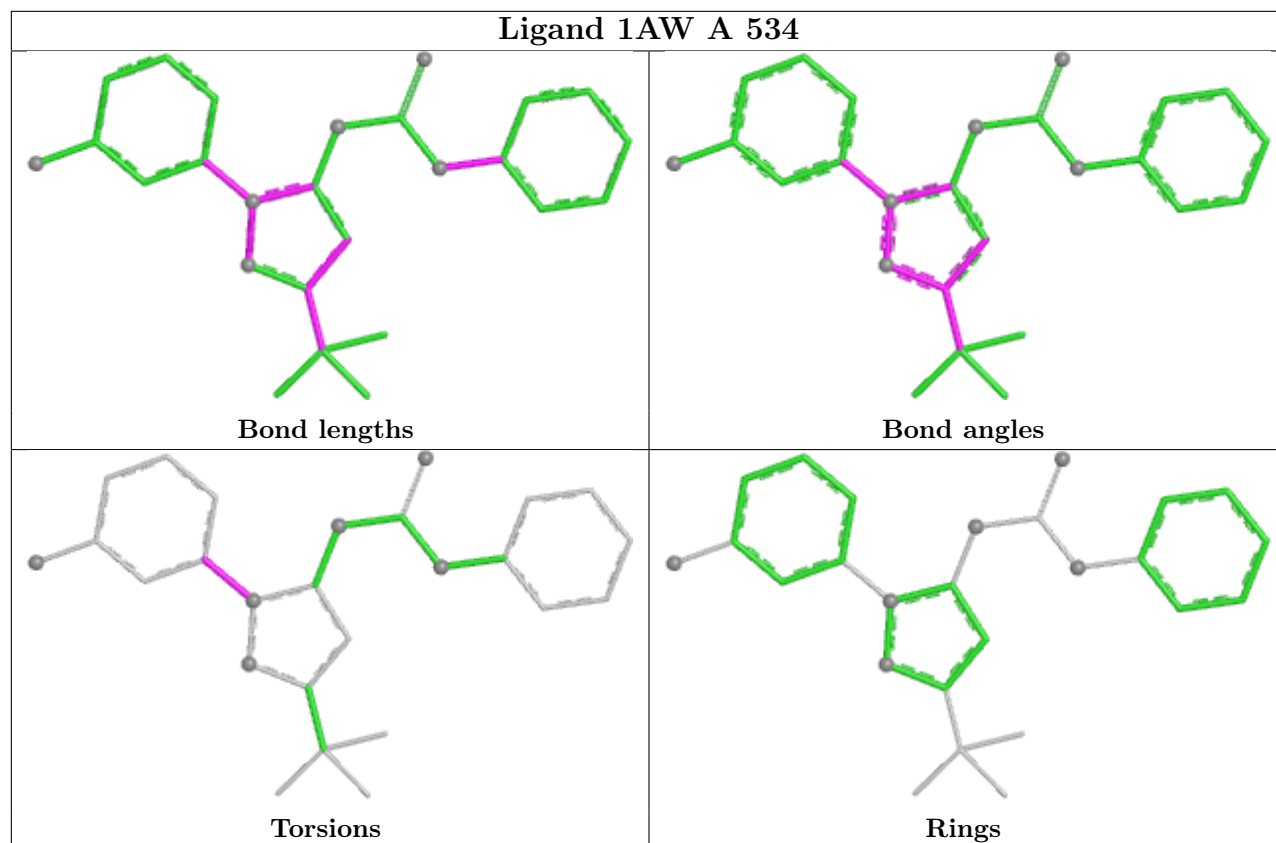
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 1AW B 1



Ligand 1AW A 1





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	261/286 (91%)	0.04	1 (0%) 88 86	2, 15, 45, 49	0
1	B	259/286 (90%)	0.31	18 (6%) 23 20	4, 15, 50, 54	0
All	All	520/572 (90%)	0.18	19 (3%) 45 40	2, 15, 48, 54	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	LEU	4.6
1	B	278	PHE	3.9
1	B	407	LEU	3.2
1	B	424	PHE	3.1
1	B	267	LEU	2.8
1	B	319	HIS	2.8
1	B	269	LEU	2.7
1	A	424	PHE	2.7
1	B	320	GLU	2.6
1	B	304	PRO	2.5
1	B	299	PRO	2.4
1	B	405	PHE	2.4
1	B	335	TYR	2.2
1	B	306	ALA	2.2
1	B	300	GLY	2.1
1	B	262	ILE	2.1
1	B	321	LYS	2.1
1	B	283	MET	2.1
1	B	334	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

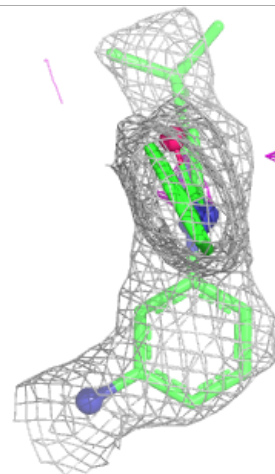
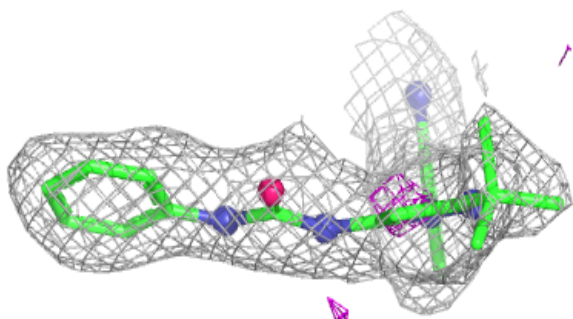
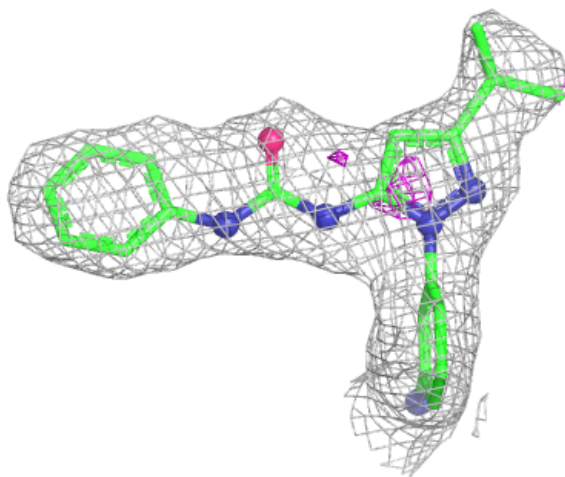
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1AW	A	534	26/26	0.84	0.15	49,54,55,55	0
2	1AW	B	1	26/26	0.84	0.16	57,63,64,64	0
2	1AW	A	1	26/26	0.90	0.10	34,35,41,43	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.

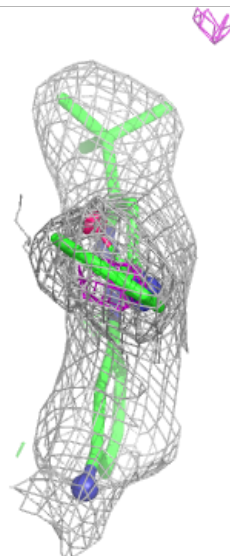
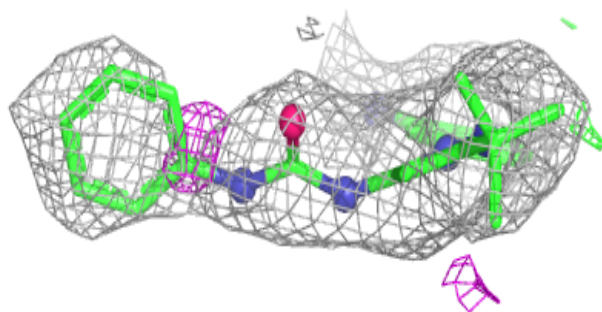
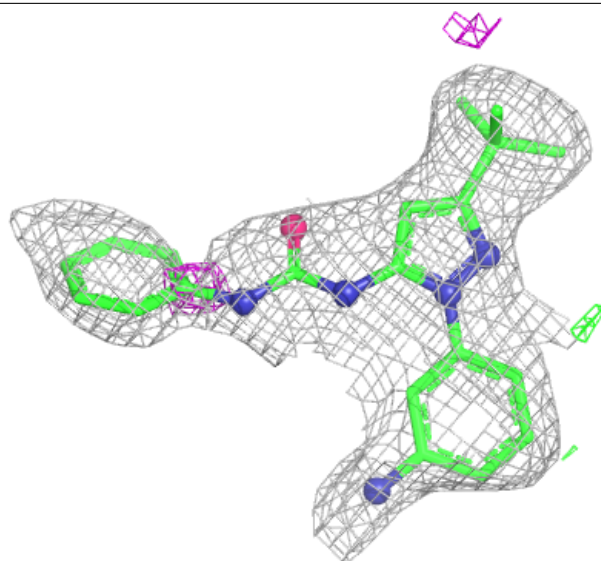
Electron density around 1AW A 534:

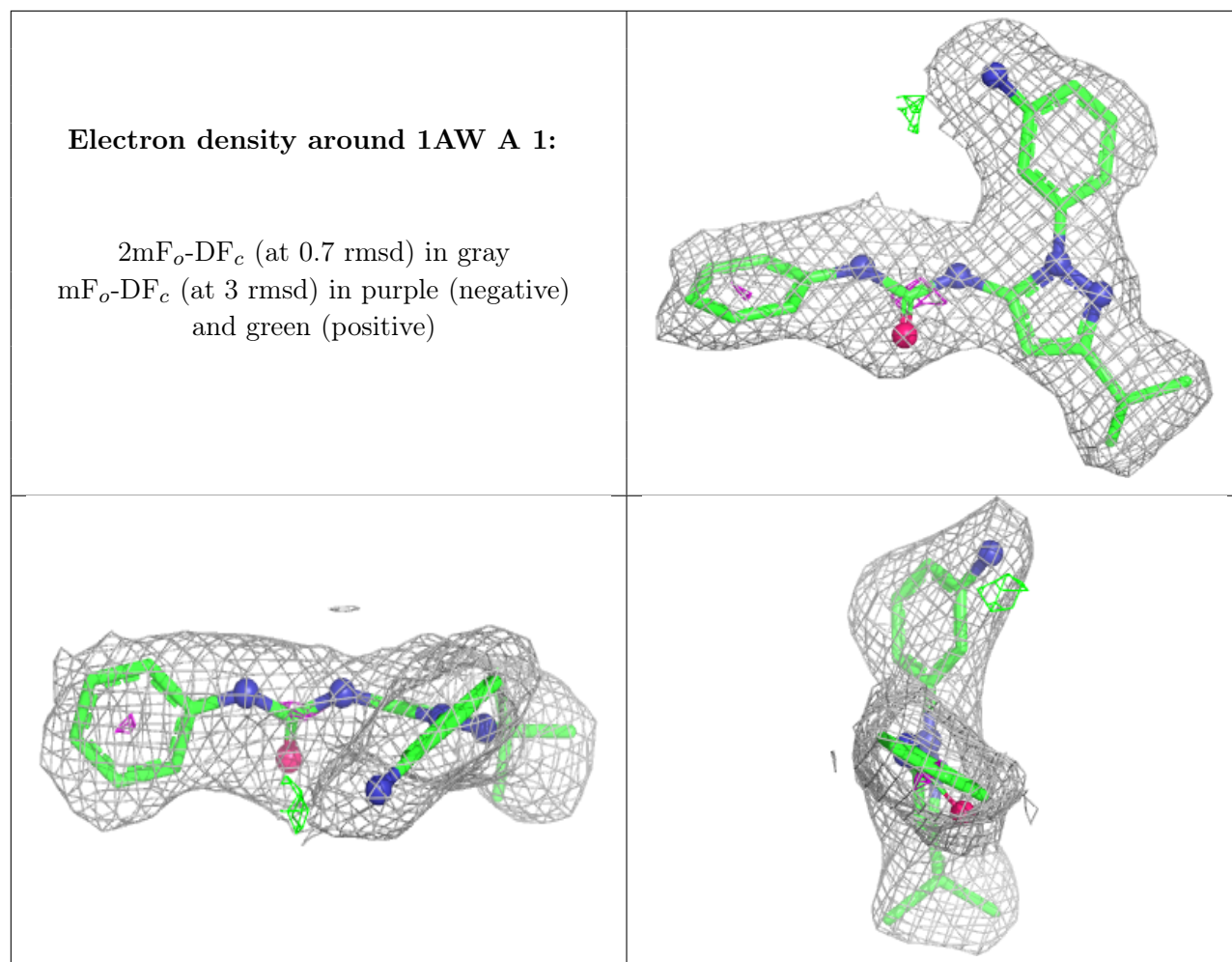
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 1AW B 1:

$2mF_o-DF_c$ (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.