



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:19 PM UTC

PDB ID : 2GTM / pdb_00002gtm
Title : Mutated Mouse P38 MAP Kinase Domain in complex with Inhibitor PG-892579
Authors : Walter, R.L.; Mekel, M.J.; Evdokimov, A.G.; Pokross, M.E.; Sabat, M.
Deposited on : 2006-04-28
Resolution : 1.90 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

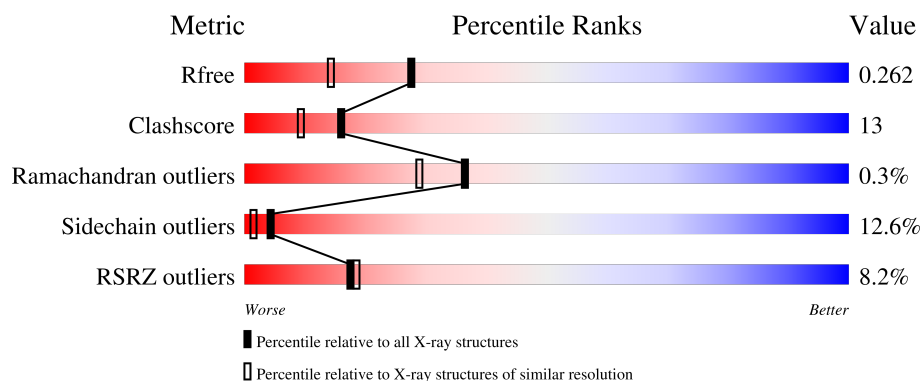
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	348	8% 68% 23% 5% ..

2 Entry composition [i](#)

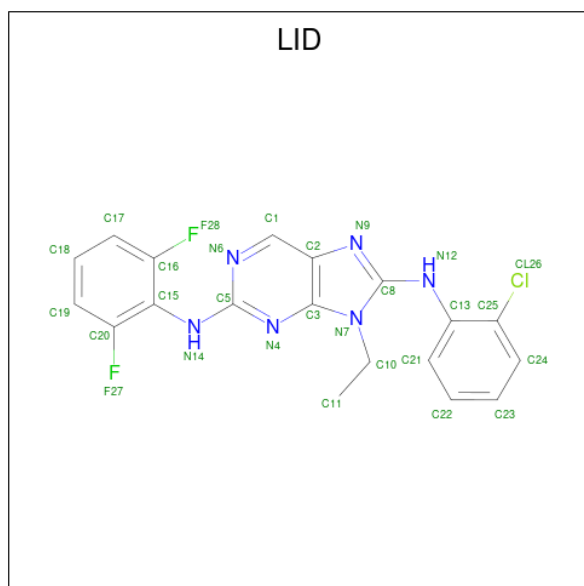
There are 3 unique types of molecules in this entry. The entry contains 2954 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2756	1767	473	505	11			

- Molecule 2 is 8-(2-CHLOROPHENYLAMINO)-2-(2,6-DIFLUOROPHENYLAMINO)-9-ETHYL-9H-PURINE-1,7-DIUM (CCD ID: LID) (formula: $C_{19}H_{15}ClF_2N_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	0	0
			28	19	1	2	6		

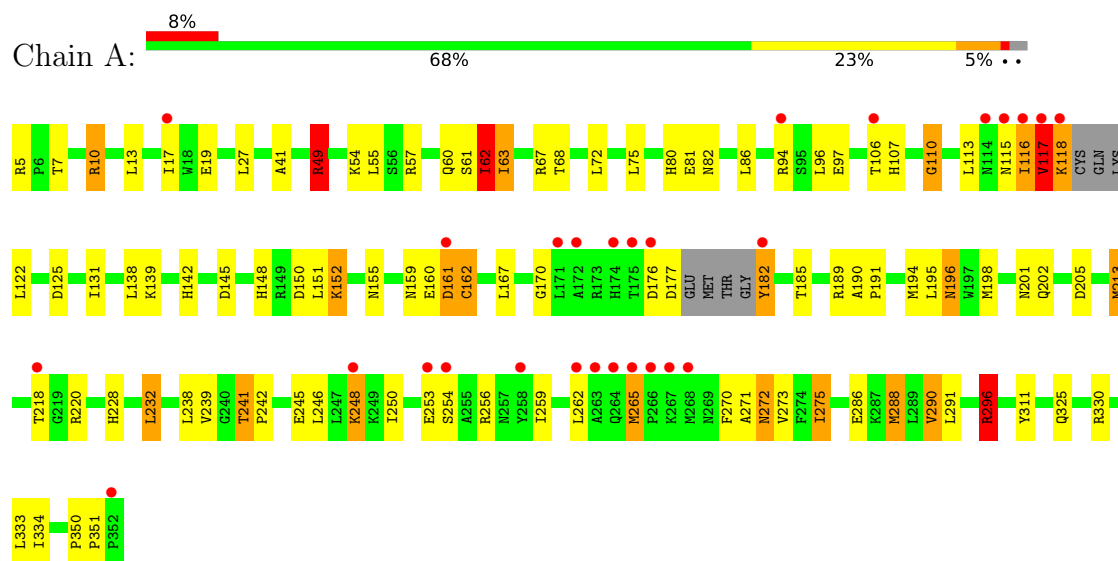
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		

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: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.88Å 73.63Å 76.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.80 – 1.90 40.80 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.80-1.90) 96.3 (40.80-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.261 0.220 , 0.262	Depositor DCC
R_{free} test set	1418 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2954	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% 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: LID

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	1.30	11/2821 (0.4%)	1.21	14/3830 (0.4%)

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	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	MET	SD-CE	-10.52	1.53	1.79
1	A	288	MET	SD-CE	-9.72	1.55	1.79
1	A	351	PRO	CA-C	9.31	1.56	1.51
1	A	182	TYR	C-N	-8.46	1.22	1.33
1	A	117	VAL	C-N	8.37	1.45	1.33
1	A	201	ASN	CA-C	7.22	1.60	1.53
1	A	62	ILE	CA-CB	6.39	1.63	1.54
1	A	296	ARG	CD-NE	-6.03	1.37	1.46
1	A	350	PRO	C-O	-5.27	1.20	1.24
1	A	117	VAL	C-O	-5.07	1.18	1.24
1	A	190	ALA	CA-CB	5.06	1.60	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	NE-CZ-NH2	-10.87	109.42	119.20
1	A	296	ARG	NE-CZ-NH1	8.03	129.53	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	LYS	CB-CG-CD	-6.61	96.09	111.30
1	A	272	ASN	CB-CA-C	-6.30	100.95	110.90
1	A	296	ARG	CD-NE-CZ	5.91	132.67	124.40
1	A	296	ARG	CG-CD-NE	-5.75	99.36	112.00
1	A	110	GLY	N-CA-C	5.70	122.92	115.40
1	A	152	LYS	N-CA-C	-5.66	103.12	108.22
1	A	250	ILE	N-CA-C	5.54	116.70	108.23
1	A	270	PHE	N-CA-C	-5.29	105.62	111.71
1	A	63	ILE	N-CA-C	5.29	116.07	110.72
1	A	159	ASN	N-CA-C	5.28	116.90	110.41
1	A	160	GLU	CA-C-N	5.07	128.79	120.63
1	A	160	GLU	C-N-CA	5.07	128.79	120.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	VAL	Mainchain
1	A	182	TYR	Mainchain
1	A	49	ARG	Sidechain

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	2756	0	2741	72	0
2	A	28	0	15	4	0
3	A	170	0	0	18	0
All	All	2954	0	2756	73	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 (73) 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:189:ARG:CD	3:A:499:HOH:O	2.02	1.04
1:A:189:ARG:HD3	3:A:499:HOH:O	1.58	1.03
1:A:202:GLN:HG3	3:A:409:HOH:O	1.66	0.95
1:A:80:HIS:HD2	1:A:82:ASN:H	1.17	0.87
1:A:152:LYS:HE3	3:A:429:HOH:O	1.88	0.73
1:A:218:THR:HG21	3:A:377:HOH:O	1.88	0.73
1:A:80:HIS:CD2	1:A:82:ASN:H	2.04	0.73
1:A:218:THR:HG23	1:A:220:ARG:H	1.54	0.72
1:A:148:HIS:HD2	1:A:150:ASP:H	1.37	0.72
1:A:290:VAL:O	1:A:296:ARG:HD3	1.91	0.71
1:A:131:ILE:HG21	1:A:213:MET:HE3	1.72	0.70
1:A:122:LEU:N	3:A:406:HOH:O	2.24	0.69
1:A:248:LYS:NZ	3:A:479:HOH:O	2.25	0.69
1:A:106:THR:HG23	1:A:107:HIS:O	1.94	0.67
1:A:107:HIS:O	2:A:353:LID:H1	1.97	0.65
1:A:241:THR:HB	3:A:522:HOH:O	1.98	0.64
1:A:262:LEU:CB	1:A:265:MET:SD	2.86	0.64
1:A:288:MET:O	1:A:296:ARG:HD2	1.98	0.63
1:A:196:ASN:HD22	1:A:198:MET:H	1.44	0.63
1:A:241:THR:HG23	1:A:265:MET:SD	2.38	0.63
1:A:272:ASN:O	1:A:275:ILE:HG13	1.99	0.63
1:A:81:GLU:H	1:A:81:GLU:CD	2.06	0.61
1:A:239:VAL:HG21	1:A:291:LEU:HD13	1.81	0.61
1:A:142:HIS:HE1	1:A:205:ASP:OD1	1.83	0.61
1:A:125:ASP:OD2	1:A:311:TYR:OH	2.17	0.60
1:A:148:HIS:HE1	1:A:167:LEU:O	1.85	0.58
1:A:262:LEU:HB3	1:A:265:MET:SD	2.43	0.58
1:A:117:VAL:N	3:A:438:HOH:O	2.36	0.58
1:A:115:ASN:HB3	3:A:474:HOH:O	2.04	0.57
1:A:17:ILE:O	1:A:54:LYS:NZ	2.28	0.56
1:A:150:ASP:OD2	1:A:185:THR:HG23	2.05	0.56
1:A:80:HIS:HE1	3:A:375:HOH:O	1.87	0.56
1:A:57:ARG:HD2	1:A:60:GLN:NE2	2.22	0.55
1:A:116:ILE:C	3:A:438:HOH:O	2.49	0.55
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.88	0.54
1:A:262:LEU:HB2	1:A:265:MET:SD	2.46	0.54
1:A:142:HIS:HD2	3:A:355:HOH:O	1.91	0.54
1:A:131:ILE:HG13	1:A:213:MET:HE3	1.88	0.54
1:A:218:THR:HG23	1:A:220:ARG:N	2.22	0.54
1:A:189:ARG:HD2	3:A:499:HOH:O	1.84	0.53
1:A:57:ARG:HD2	1:A:60:GLN:HE22	1.74	0.50
1:A:110:GLY:H	2:A:353:LID:H14	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:CG2	1:A:220:ARG:H	2.25	0.49
1:A:271:ALA:O	1:A:275:ILE:HG23	2.12	0.49
1:A:75:LEU:HD11	2:A:353:LID:H22	1.94	0.48
1:A:115:ASN:C	1:A:117:VAL:H	2.23	0.47
1:A:155:ASN:ND2	1:A:170:GLY:N	2.63	0.46
1:A:10:ARG:HH22	1:A:17:ILE:HD13	1.81	0.46
1:A:27:LEU:HD23	1:A:41:ALA:HB2	1.98	0.46
1:A:61:SER:HA	1:A:334:ILE:HD11	1.98	0.45
1:A:161:ASP:O	1:A:162:CYS:CB	2.64	0.45
1:A:55:LEU:HD12	1:A:68:THR:HG23	1.99	0.44
1:A:62:ILE:HG22	1:A:334:ILE:HG13	1.99	0.44
1:A:202:GLN:CG	3:A:409:HOH:O	2.43	0.44
1:A:238:LEU:CD1	1:A:273:VAL:HG21	2.48	0.44
1:A:75:LEU:HB3	1:A:86:LEU:HG	2.00	0.44
1:A:10:ARG:CG	1:A:19:GLU:HG2	2.48	0.43
1:A:139:LYS:NZ	3:A:411:HOH:O	2.51	0.43
1:A:191:PRO:HG3	1:A:291:LEU:HD12	2.01	0.43
1:A:194:MET:HG2	1:A:232:LEU:CD2	2.48	0.43
1:A:290:VAL:O	1:A:296:ARG:CD	2.63	0.43
1:A:253:GLU:HG3	1:A:256:ARG:HH22	1.84	0.42
1:A:228:HIS:O	1:A:232:LEU:CD2	2.68	0.42
1:A:262:LEU:O	1:A:265:MET:HE2	2.20	0.42
1:A:262:LEU:HB3	1:A:265:MET:HE2	2.01	0.41
1:A:10:ARG:HG3	1:A:19:GLU:HG2	2.02	0.41
1:A:241:THR:HG22	1:A:242:PRO:HD2	2.03	0.41
1:A:241:THR:CG2	1:A:265:MET:SD	3.06	0.41
2:A:353:LID:H112	3:A:405:HOH:O	2.20	0.41
1:A:49:ARG:NE	3:A:417:HOH:O	2.54	0.40
1:A:131:ILE:CG2	1:A:213:MET:HE3	2.48	0.40
1:A:155:ASN:HD21	1:A:170:GLY:H	1.69	0.40
1:A:194:MET:HG2	1:A:232:LEU:HD22	2.03	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	335/348 (96%)	323 (96%)	11 (3%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ILE

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	301/307 (98%)	263 (87%)	38 (13%)	4	1

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	7	THR
1	A	10	ARG
1	A	13	LEU
1	A	49	ARG
1	A	62	ILE
1	A	63	ILE
1	A	67	ARG
1	A	72	LEU
1	A	94	ARG
1	A	96	LEU
1	A	97	GLU
1	A	113	LEU
1	A	117	VAL
1	A	118	LYS
1	A	138	LEU
1	A	145	ASP
1	A	151	LEU

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Mol	Chain	Res	Type
1	A	161	ASP
1	A	162	CYS
1	A	176	ASP
1	A	177	ASP
1	A	195	LEU
1	A	196	ASN
1	A	232	LEU
1	A	241	THR
1	A	245	GLU
1	A	248	LYS
1	A	254	SER
1	A	259	ILE
1	A	265	MET
1	A	275	ILE
1	A	286	GLU
1	A	290	VAL
1	A	296	ARG
1	A	325	GLN
1	A	330	ARG
1	A	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	64	HIS
1	A	80	HIS
1	A	107	HIS
1	A	126	HIS
1	A	128	GLN
1	A	142	HIS
1	A	148	HIS
1	A	196	ASN
1	A	202	GLN
1	A	257	ASN
1	A	260	GLN
1	A	310	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](#)

1 ligand is 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	LID	A	353	-	30,31,31	3.89	16 (53%)	37,44,44	2.72	12 (32%)

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	LID	A	353	-	-	3/10/10/10	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	353	LID	C5-N6	9.53	1.47	1.34
2	A	353	LID	C23-C24	9.37	1.54	1.38
2	A	353	LID	C15-C16	7.78	1.50	1.38
2	A	353	LID	C23-C22	7.22	1.54	1.38
2	A	353	LID	C1-C2	5.53	1.47	1.39
2	A	353	LID	C8-N9	4.52	1.39	1.32
2	A	353	LID	C3-N7	-4.36	1.29	1.39
2	A	353	LID	C5-N4	3.77	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	353	LID	C21-C13	-3.34	1.34	1.39
2	A	353	LID	C2-C3	-3.34	1.34	1.40
2	A	353	LID	C5-N14	3.09	1.43	1.36
2	A	353	LID	C15-N14	-2.97	1.32	1.41
2	A	353	LID	C22-C21	-2.87	1.34	1.38
2	A	353	LID	C13-C25	-2.39	1.34	1.39
2	A	353	LID	C18-C17	2.35	1.42	1.38
2	A	353	LID	C1-N6	-2.01	1.30	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	353	LID	C22-C23-C24	-7.13	111.44	120.24
2	A	353	LID	C16-C15-C20	5.94	122.14	115.70
2	A	353	LID	N6-C5-N4	-5.65	120.95	126.42
2	A	353	LID	C17-C16-C15	-5.34	115.18	122.83
2	A	353	LID	C1-C2-C3	5.32	122.05	116.24
2	A	353	LID	F28-C16-C15	5.15	122.99	117.64
2	A	353	LID	C20-C15-N14	-3.61	116.38	122.00
2	A	353	LID	C2-C3-N4	-3.20	122.22	126.55
2	A	353	LID	C24-C25-C13	2.61	125.16	121.48
2	A	353	LID	C22-C21-C13	2.38	123.53	118.69
2	A	353	LID	C3-C2-N9	-2.21	108.07	110.34
2	A	353	LID	C21-C13-C25	2.02	120.60	117.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	353	LID	C11-C10-N7-C3
2	A	353	LID	C25-C13-N12-C8
2	A	353	LID	C11-C10-N7-C8

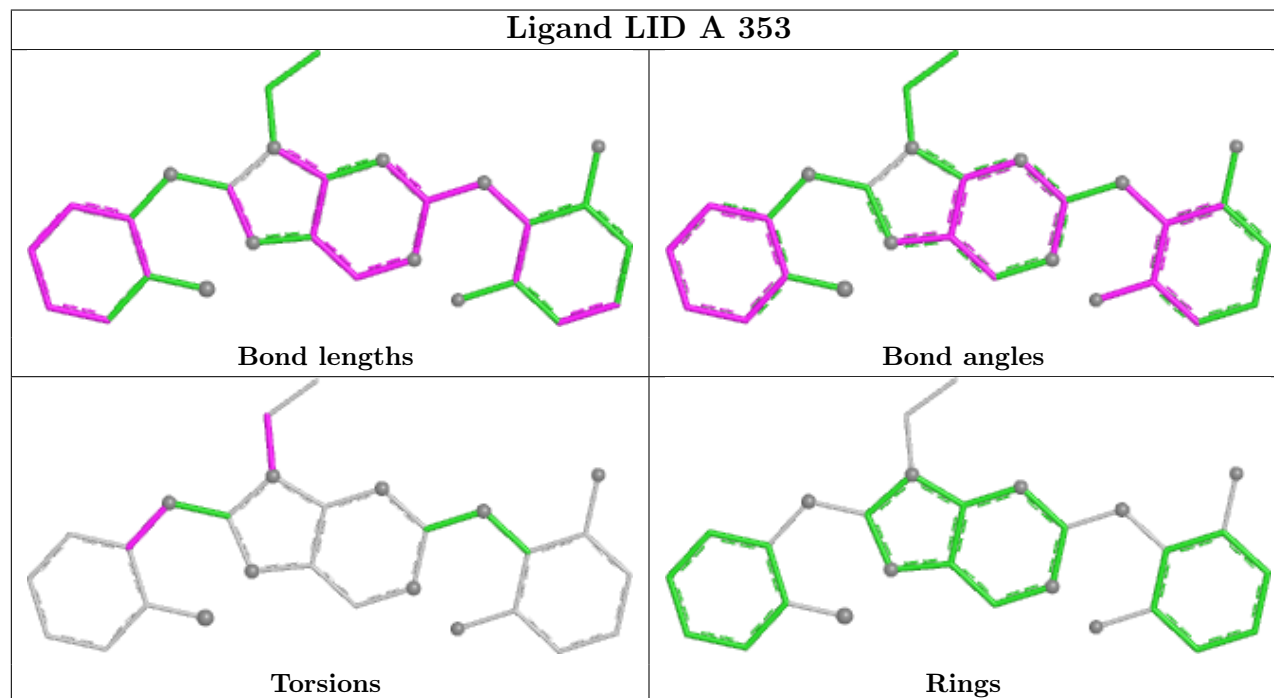
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	353	LID	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.



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	341/348 (97%)	0.70	28 (8%) 17 18	20, 36, 59, 78	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	ALA	6.7
1	A	262	LEU	5.7
1	A	182	TYR	5.5
1	A	258	TYR	5.1
1	A	118	LYS	4.8
1	A	117	VAL	4.8
1	A	116	ILE	4.6
1	A	265	MET	3.6
1	A	266	PRO	3.4
1	A	268	MET	3.2
1	A	171	LEU	2.9
1	A	248	LYS	2.6
1	A	161	ASP	2.6
1	A	175	THR	2.6
1	A	17	ILE	2.5
1	A	174	HIS	2.5
1	A	218	THR	2.5
1	A	254	SER	2.4
1	A	264	GLN	2.4
1	A	106	THR	2.3
1	A	176	ASP	2.3
1	A	115	ASN	2.3
1	A	352	PRO	2.2
1	A	267	LYS	2.2
1	A	253	GLU	2.1
1	A	172	ALA	2.1
1	A	94	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	114	ASN	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](#)

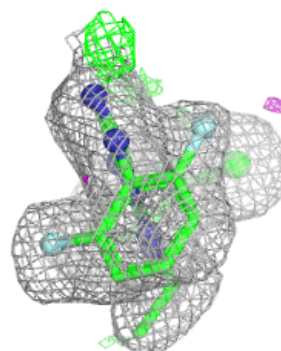
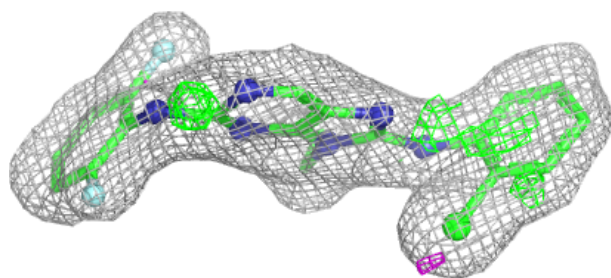
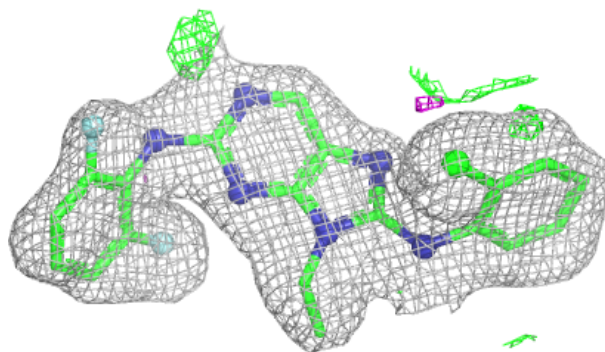
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LID	A	353	28/28	0.91	0.09	26,34,42,48	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 LID A 353:

$2mF_o-DF_c$ (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.