



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:48 AM EDT

PDB ID : 2GTN / pdb_00002gtn
Title : Mutated MAP kinase P38 (Mus Musculus) in complex with Inhibitor PG-951717
Authors : Walter, R.L.; Mekel, M.J.; Evdokimov, A.G.; Pokross, M.E.; Sabat, M.
Deposited on : 2006-04-28
Resolution : 1.80 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

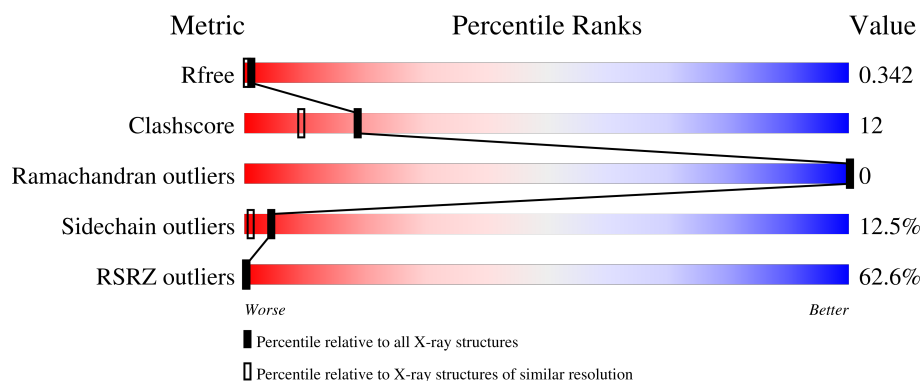
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2972 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.

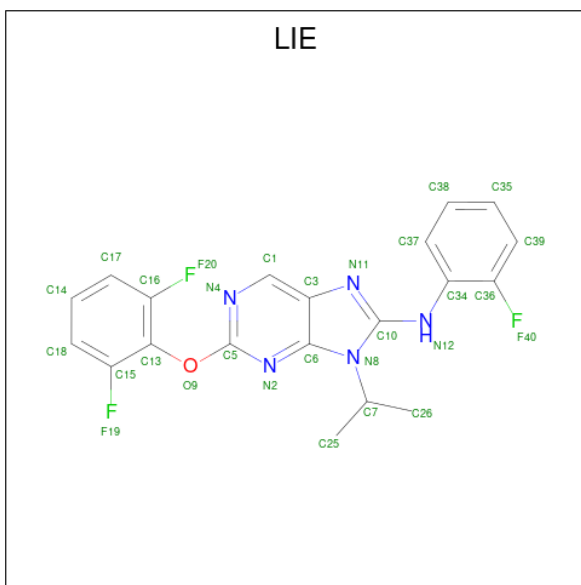
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2717	1743	466	496	12	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is 2-(2,6-DIFLUOROPHENOXY)-N-(2-FLUOROPHENYL)-9-ISOPROPYL-9H-PURIN-8-AMINE (CCD ID: LIE) (formula: C₂₀H₁₆F₃N₅O).



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

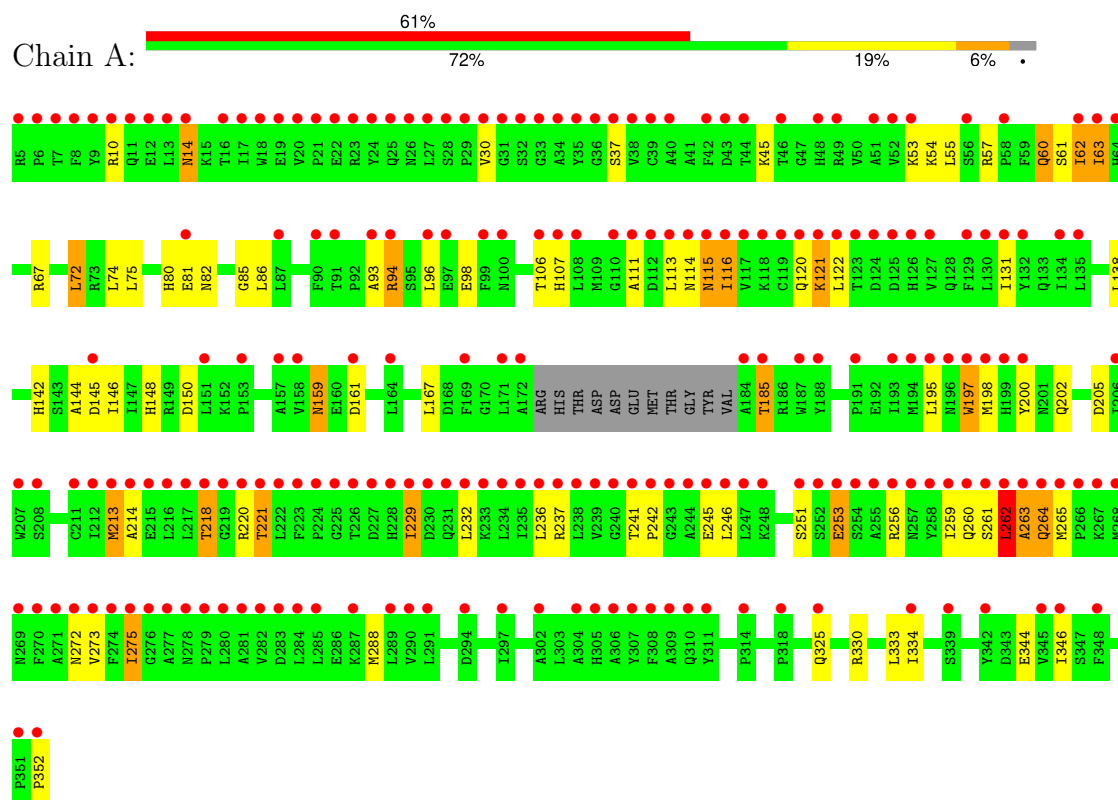
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		

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	64.99Å 74.55Å 78.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.81	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-1.80) 95.3 (50.00-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.82Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.248 0.319 , 0.342	Depositor DCC
R_{free} test set	1678 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2972	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: SO4, LIE

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	1.14	4/2781 (0.1%)	1.10	7/3775 (0.2%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	MET	SD-CE	-13.04	1.47	1.79
1	A	262	LEU	N-CA	-12.00	1.30	1.46
1	A	213	MET	SD-CE	-10.06	1.54	1.79
1	A	262	LEU	C-N	-6.70	1.25	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	LEU	N-CA-C	-11.22	86.90	110.80
1	A	262	LEU	CA-C-N	-7.65	112.46	121.64
1	A	262	LEU	C-N-CA	-7.65	112.46	121.64
1	A	221	THR	CB-CA-C	5.57	118.81	109.89
1	A	30	VAL	N-CA-C	-5.50	106.44	111.67
1	A	263	ALA	CA-C-O	5.37	123.49	119.68
1	A	121	LYS	N-CA-C	5.29	116.57	108.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2717	0	2715	63	0
2	A	5	0	0	1	0
3	A	29	0	16	2	0
4	A	221	0	0	24	0
All	All	2972	0	2731	65	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 12.

All (65) 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:111:ALA:HB1	1:A:115:ASN:HD21	1.03	1.18
1:A:111:ALA:HB1	1:A:115:ASN:ND2	1.87	0.89
1:A:80:HIS:HD2	1:A:82:ASN:H	1.21	0.88
1:A:53:LYS:HG2	4:A:556:HOH:O	1.74	0.86
1:A:107:HIS:ND1	2:A:353:SO4:O4	2.13	0.80
1:A:81:GLU:HG2	4:A:396:HOH:O	1.84	0.77
1:A:98:GLU:HB2	4:A:507:HOH:O	1.85	0.77
1:A:63:ILE:HD11	1:A:67:ARG:NH2	2.03	0.74
1:A:115:ASN:C	1:A:115:ASN:HD22	1.95	0.73
1:A:75:LEU:HB3	1:A:86:LEU:HG	1.73	0.70
1:A:218:THR:HG22	1:A:220:ARG:H	1.56	0.70
1:A:272:ASN:O	1:A:275:ILE:HG12	1.92	0.69
1:A:218:THR:HG21	4:A:377:HOH:O	1.92	0.69
1:A:261:SER:C	1:A:262:LEU:O	2.29	0.68
1:A:86:LEU:HD23	4:A:565:HOH:O	1.94	0.67
3:A:354:LIE:H35	4:A:565:HOH:O	1.94	0.67
1:A:148:HIS:HD2	1:A:150:ASP:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:HD2	1:A:60:GLN:HE22	1.60	0.66
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.77	0.66
1:A:81:GLU:CG	4:A:396:HOH:O	2.43	0.64
1:A:55:LEU:HD23	4:A:556:HOH:O	1.97	0.63
1:A:55:LEU:HA	4:A:556:HOH:O	1.98	0.62
1:A:106:THR:HG23	4:A:565:HOH:O	2.00	0.62
1:A:197:TRP:HD1	1:A:200:TYR:CE1	2.18	0.61
1:A:80:HIS:CD2	1:A:82:ASN:H	2.11	0.60
1:A:159:ASN:C	1:A:159:ASN:HD22	2.09	0.60
1:A:94:ARG:HG2	4:A:575:HOH:O	2.01	0.60
1:A:214:ALA:O	1:A:218:THR:HB	2.00	0.60
1:A:115:ASN:ND2	1:A:115:ASN:O	2.33	0.60
1:A:148:HIS:HE1	1:A:167:LEU:O	1.85	0.58
1:A:352:PRO:O	4:A:523:HOH:O	2.17	0.58
1:A:142:HIS:HD2	4:A:360:HOH:O	1.87	0.56
1:A:218:THR:CG2	1:A:220:ARG:H	2.20	0.55
1:A:344:GLU:C	4:A:569:HOH:O	2.50	0.54
1:A:57:ARG:HD2	1:A:60:GLN:NE2	2.23	0.54
1:A:325:GLN:NE2	4:A:438:HOH:O	2.40	0.53
1:A:93:ALA:HA	4:A:507:HOH:O	2.11	0.50
1:A:232:LEU:HD21	1:A:259:ILE:HG12	1.94	0.50
1:A:144:ALA:HB3	1:A:146:ILE:HD12	1.92	0.50
1:A:145:ASP:OD1	4:A:554:HOH:O	2.20	0.50
1:A:131:ILE:HG13	1:A:213:MET:HE3	1.93	0.50
1:A:253:GLU:CD	1:A:256:ARG:HH22	2.19	0.50
1:A:14:ASN:OD1	1:A:14:ASN:N	2.45	0.50
1:A:80:HIS:HE1	4:A:363:HOH:O	1.94	0.50
1:A:85:GLY:O	1:A:106:THR:HG22	2.12	0.50
1:A:142:HIS:HE1	1:A:205:ASP:OD1	1.94	0.50
1:A:197:TRP:HD1	1:A:200:TYR:CZ	2.30	0.49
1:A:236:LEU:HD12	1:A:262:LEU:HD13	1.93	0.49
1:A:264:GLN:HG3	1:A:265:MET:N	2.28	0.48
1:A:237:ARG:HD2	4:A:548:HOH:O	2.13	0.48
1:A:72:LEU:HD11	4:A:569:HOH:O	2.14	0.48
1:A:61:SER:HA	1:A:334:ILE:HD11	1.97	0.47
1:A:54:LYS:C	4:A:556:HOH:O	2.57	0.46
1:A:62:ILE:HG22	1:A:334:ILE:HG13	1.98	0.46
1:A:242:PRO:HG3	1:A:259:ILE:HG21	1.98	0.46
1:A:198:MET:SD	1:A:251:SER:OG	2.74	0.44
1:A:150:ASP:OD2	1:A:185:THR:HG23	2.17	0.43
1:A:272:ASN:O	1:A:275:ILE:CG1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:O	1:A:116:ILE:CG2	2.67	0.43
1:A:253:GLU:H	1:A:253:GLU:HG2	1.64	0.43
1:A:202:GLN:NE2	4:A:554:HOH:O	2.51	0.42
1:A:94:ARG:CZ	1:A:94:ARG:HB3	2.49	0.42
1:A:260:GLN:C	4:A:432:HOH:O	2.62	0.42
3:A:354:LIE:C35	4:A:565:HOH:O	2.60	0.41
1:A:229:ILE:C	1:A:229:ILE:HD12	2.46	0.41

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	333/348 (96%)	324 (97%)	9 (3%)	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	297/307 (97%)	260 (88%)	37 (12%)	4	1

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	14	ASN
1	A	37	SER
1	A	45	LYS
1	A	60	GLN
1	A	62	ILE
1	A	63	ILE
1	A	72	LEU
1	A	74	LEU
1	A	94	ARG
1	A	96	LEU
1	A	113	LEU
1	A	114	ASN
1	A	115	ASN
1	A	116	ILE
1	A	120	GLN
1	A	121	LYS
1	A	122	LEU
1	A	138	LEU
1	A	159	ASN
1	A	161	ASP
1	A	185	THR
1	A	195	LEU
1	A	197	TRP
1	A	218	THR
1	A	221	THR
1	A	229	ILE
1	A	241	THR
1	A	245	GLU
1	A	253	GLU
1	A	262	LEU
1	A	264	GLN
1	A	273	VAL
1	A	275	ILE
1	A	330	ARG
1	A	333	LEU
1	A	346	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	60	GLN

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Mol	Chain	Res	Type
1	A	64	HIS
1	A	80	HIS
1	A	114	ASN
1	A	115	ASN
1	A	120	GLN
1	A	126	HIS
1	A	142	HIS
1	A	148	HIS
1	A	159	ASN
1	A	228	HIS
1	A	257	ASN
1	A	260	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	LIE	A	354	-	32,32,32	1.45	3 (9%)	40,46,46	2.03	13 (32%)
2	SO4	A	353	-	4,4,4	0.53	0	6,6,6	0.63	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	LIE	A	354	-	-	0/12/12/12	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	LIE	C6-N8	-5.29	1.30	1.38
3	A	354	LIE	C5-N4	2.97	1.36	1.32
3	A	354	LIE	C3-C6	-2.34	1.36	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	354	LIE	N4-C5-N2	-5.85	123.31	128.35
3	A	354	LIE	C3-C6-N2	-4.73	120.16	126.55
3	A	354	LIE	C37-C34-C36	3.64	121.21	117.23
3	A	354	LIE	N8-C10-N11	3.47	116.98	114.42
3	A	354	LIE	C7-N8-C10	3.04	130.35	123.94
3	A	354	LIE	C3-N11-C10	-3.02	99.36	104.06
3	A	354	LIE	C1-C3-C6	2.57	119.05	116.24
3	A	354	LIE	C3-C6-N8	2.42	111.14	106.78
3	A	354	LIE	F19-C15-C18	2.39	124.19	118.65
3	A	354	LIE	F40-C36-C34	2.28	120.43	117.59
3	A	354	LIE	O9-C13-C15	-2.15	117.51	121.06
3	A	354	LIE	C1-N4-C5	2.09	117.42	115.00
3	A	354	LIE	C39-C36-C34	-2.05	120.88	123.18

There are no chirality outliers.

There are no torsion outliers.

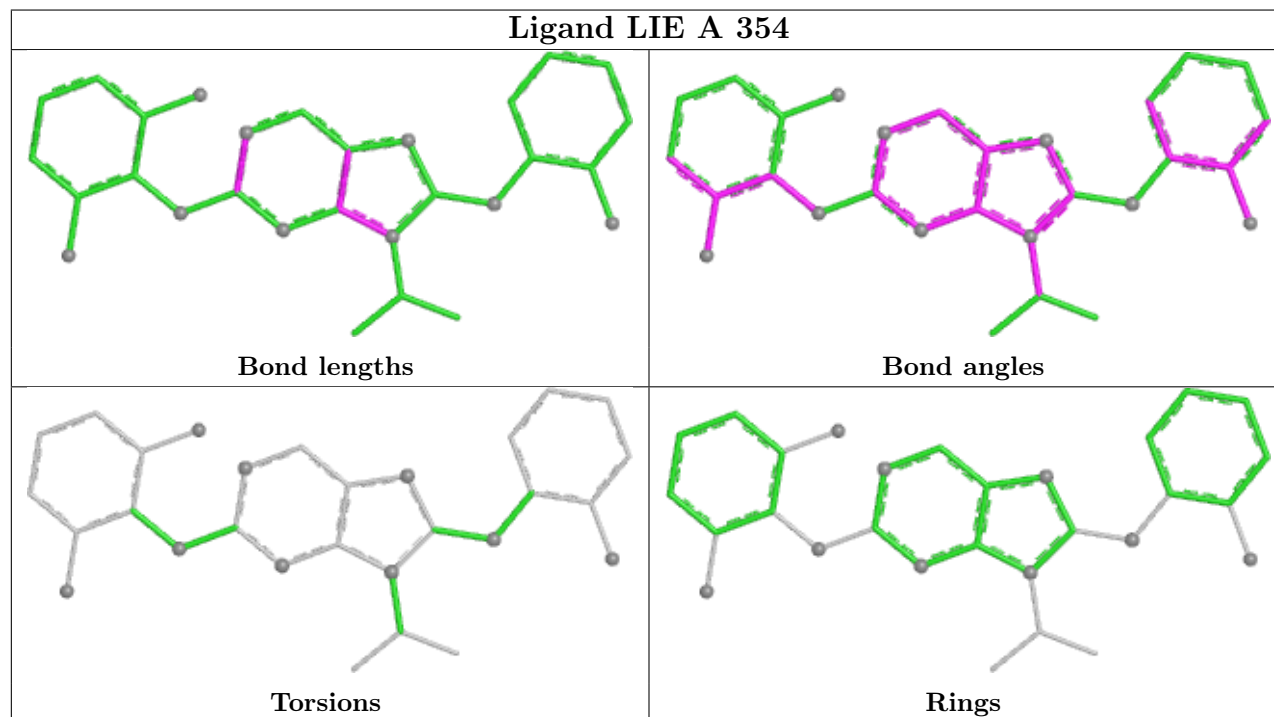
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	354	LIE	2	0
2	A	353	SO4	1	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	337/348 (96%)	2.64	211 (62%) 0 0	19, 33, 53, 77	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	THR	7.8
1	A	172	ALA	6.9
1	A	219	GLY	6.8
1	A	117	VAL	6.6
1	A	17	ILE	6.6
1	A	262	LEU	6.5
1	A	116	ILE	6.4
1	A	275	ILE	6.0
1	A	271	ALA	6.0
1	A	115	ASN	6.0
1	A	238	LEU	5.9
1	A	42	PHE	5.8
1	A	229	ILE	5.6
1	A	268	MET	5.6
1	A	276	GLY	5.5
1	A	35	TYR	5.5
1	A	263	ALA	5.4
1	A	266	PRO	5.3
1	A	290	VAL	5.0
1	A	123	THR	4.9
1	A	274	PHE	4.9
1	A	273	VAL	4.9
1	A	282	VAL	4.9
1	A	280	LEU	4.8
1	A	197	TRP	4.7
1	A	225	GLY	4.7
1	A	239	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	221	THR	4.7
1	A	111	ALA	4.6
1	A	243	GLY	4.6
1	A	13	LEU	4.6
1	A	217	LEU	4.6
1	A	112	ASP	4.6
1	A	161	ASP	4.5
1	A	281	ALA	4.5
1	A	232	LEU	4.5
1	A	18	TRP	4.4
1	A	9	TYR	4.4
1	A	185	THR	4.4
1	A	240	GLY	4.4
1	A	302	ALA	4.4
1	A	113	LEU	4.3
1	A	28	SER	4.3
1	A	122	LEU	4.3
1	A	272	ASN	4.3
1	A	40	ALA	4.3
1	A	255	ALA	4.3
1	A	234	LEU	4.2
1	A	244	ALA	4.1
1	A	258	TYR	4.1
1	A	44	THR	4.1
1	A	261	SER	4.1
1	A	277	ALA	4.1
1	A	49	ARG	4.1
1	A	33	GLY	4.1
1	A	169	PHE	4.0
1	A	236	LEU	4.0
1	A	119	CYS	4.0
1	A	20	VAL	4.0
1	A	265	MET	4.0
1	A	187	TRP	4.0
1	A	125	ASP	3.9
1	A	267	LYS	3.9
1	A	171	LEU	3.9
1	A	14	ASN	3.8
1	A	30	VAL	3.8
1	A	27	LEU	3.7
1	A	100	ASN	3.7
1	A	270	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	224	PRO	3.7
1	A	230	ASP	3.7
1	A	223	PHE	3.7
1	A	38	VAL	3.7
1	A	158	VAL	3.7
1	A	29	PRO	3.7
1	A	247	LEU	3.6
1	A	48	HIS	3.6
1	A	118	LYS	3.6
1	A	231	GLN	3.6
1	A	32	SER	3.6
1	A	278	ASN	3.5
1	A	310	GLN	3.5
1	A	279	PRO	3.5
1	A	96	LEU	3.5
1	A	164	LEU	3.5
1	A	246	LEU	3.5
1	A	31	GLY	3.5
1	A	352	PRO	3.4
1	A	194	MET	3.4
1	A	126	HIS	3.4
1	A	37	SER	3.4
1	A	19	GLU	3.4
1	A	26	ASN	3.4
1	A	114	ASN	3.4
1	A	107	HIS	3.4
1	A	51	ALA	3.4
1	A	7	THR	3.4
1	A	121	LYS	3.3
1	A	237	ARG	3.3
1	A	259	ILE	3.3
1	A	309	ALA	3.3
1	A	211	CYS	3.3
1	A	213	MET	3.2
1	A	8	PHE	3.2
1	A	218	THR	3.2
1	A	222	LEU	3.2
1	A	285	LEU	3.2
1	A	308	PHE	3.2
1	A	307	TYR	3.1
1	A	200	TYR	3.1
1	A	226	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	ASP	3.1
1	A	216	LEU	3.1
1	A	12	GLU	3.1
1	A	235	ILE	3.0
1	A	23	ARG	3.0
1	A	6	PRO	3.0
1	A	242	PRO	3.0
1	A	157	ALA	3.0
1	A	63	ILE	3.0
1	A	52	VAL	3.0
1	A	199	HIS	3.0
1	A	220	ARG	3.0
1	A	11	GLN	2.9
1	A	46	THR	2.9
1	A	257	ASN	2.9
1	A	130	LEU	2.9
1	A	264	GLN	2.8
1	A	291	LEU	2.8
1	A	120	GLN	2.8
1	A	135	LEU	2.8
1	A	228	HIS	2.8
1	A	129	PHE	2.8
1	A	196	ASN	2.8
1	A	269	ASN	2.8
1	A	212	ILE	2.8
1	A	254	SER	2.7
1	A	93	ALA	2.7
1	A	106	THR	2.7
1	A	241	THR	2.7
1	A	294	ASP	2.7
1	A	297	ILE	2.7
1	A	346	ILE	2.7
1	A	97	GLU	2.7
1	A	184	ALA	2.7
1	A	314	PRO	2.7
1	A	253	GLU	2.7
1	A	260	GLN	2.7
1	A	193	ILE	2.7
1	A	195	LEU	2.6
1	A	131	ILE	2.6
1	A	311	TYR	2.6
1	A	304	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	39	CYS	2.6
1	A	90	PHE	2.6
1	A	108	LEU	2.6
1	A	151	LEU	2.6
1	A	198	MET	2.6
1	A	110	GLY	2.6
1	A	345	VAL	2.6
1	A	58	PRO	2.5
1	A	43	ASP	2.5
1	A	334	ILE	2.5
1	A	227	ASP	2.5
1	A	289	LEU	2.5
1	A	81	GLU	2.5
1	A	191	PRO	2.5
1	A	215	GLU	2.4
1	A	188	TYR	2.4
1	A	62	ILE	2.4
1	A	206	ILE	2.4
1	A	124	ASP	2.3
1	A	245	GLU	2.3
1	A	25	GLN	2.3
1	A	99	PHE	2.3
1	A	348	PHE	2.3
1	A	214	ALA	2.3
1	A	24	TYR	2.3
1	A	233	LYS	2.3
1	A	256	ARG	2.3
1	A	252	SER	2.3
1	A	248	LYS	2.3
1	A	306	ALA	2.2
1	A	208	SER	2.2
1	A	10	ARG	2.2
1	A	284	LEU	2.2
1	A	56	SER	2.2
1	A	251	SER	2.2
1	A	318	PRO	2.2
1	A	339	SER	2.2
1	A	132	TYR	2.2
1	A	94	ARG	2.2
1	A	36	GLY	2.2
1	A	283	ASP	2.2
1	A	287	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	21	PRO	2.2
1	A	351	PRO	2.2
1	A	5	ARG	2.2
1	A	64	HIS	2.1
1	A	207	TRP	2.1
1	A	22	GLU	2.1
1	A	305	HIS	2.1
1	A	134	ILE	2.1
1	A	342	TYR	2.1
1	A	91	THR	2.1
1	A	87	LEU	2.1
1	A	53	LYS	2.1
1	A	153	PRO	2.1
1	A	325	GLN	2.1
1	A	127	VAL	2.0
1	A	34	ALA	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](#)

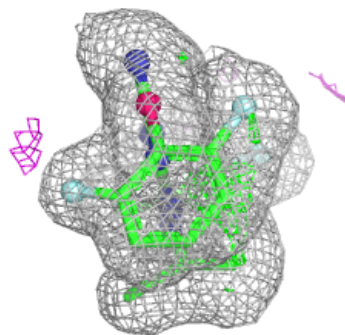
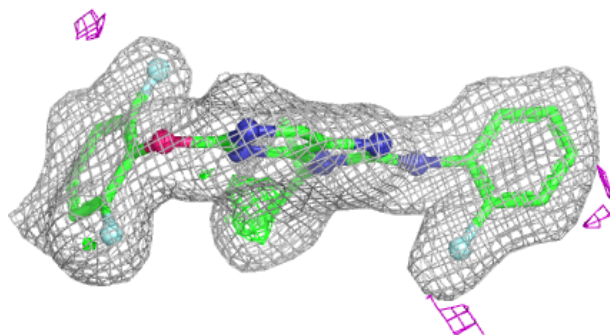
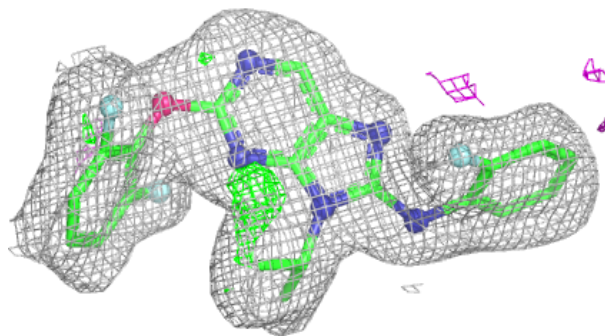
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	353	5/5	0.77	0.17	45,47,49,52	0
3	LIE	A	354	29/29	0.85	0.12	21,26,33,35	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 LIE A 354:

$2mF_o - DF_c$ (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.