



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:28 PM UTC

PDB ID : 5A9U / pdb_00005a9u
Title : Structure of C1156Y Mutant Human Anaplastic Lymphoma Kinase in Complex with PF-06463922 ((10R)-7-amino-12-fluoro-2,10,16-trimethyl- 15-oxo-10,15,16,17-tetrahydro-2H-8,4-(metheno)pyrazolo(4,3-h)(2,5,11) benzoxadiazacyclotetradecine-3-carbonitrile).
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Deposited on : 2015-07-22
Resolution : 1.60 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](#) ①) 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

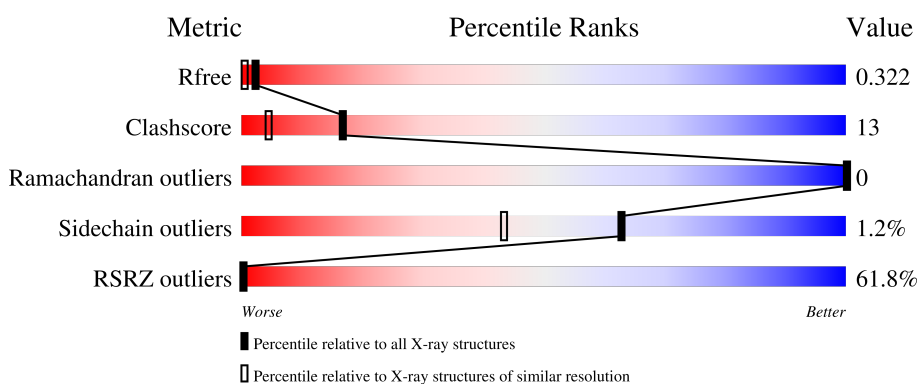
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	327	55% 73%16%10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2558 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.

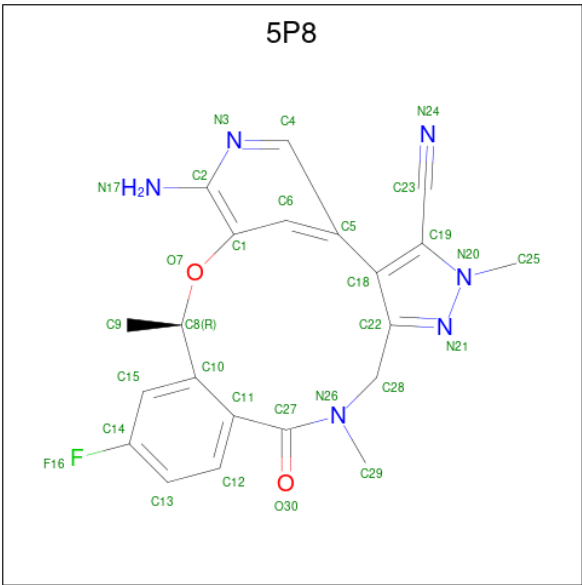
- Molecule 1 is a protein called ALK TYROSINE KINASE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2330	1485	397	426	22	0	3	1

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	MET	-	expression tag	UNP Q9UM73
A	1086	ALA	-	expression tag	UNP Q9UM73
A	1087	HIS	-	expression tag	UNP Q9UM73
A	1088	HIS	-	expression tag	UNP Q9UM73
A	1089	HIS	-	expression tag	UNP Q9UM73
A	1090	HIS	-	expression tag	UNP Q9UM73
A	1091	HIS	-	expression tag	UNP Q9UM73
A	1092	HIS	-	expression tag	UNP Q9UM73
A	1156	TYR	CYS	engineered mutation	UNP Q9UM73

- Molecule 2 is (10R)-7-amino-12-fluoro-2,10,16-trimethyl-15-oxo-10,15,16,17-tetrahydro-2H-8,4-(metheno)pyrazolo[4,3-h][2,5,11]benzoxadiazacyclotetradecine-3-carbonitrile (CCD ID: 5P8) (formula: C₂₁H₁₉FN₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			30	21	1	6	2		

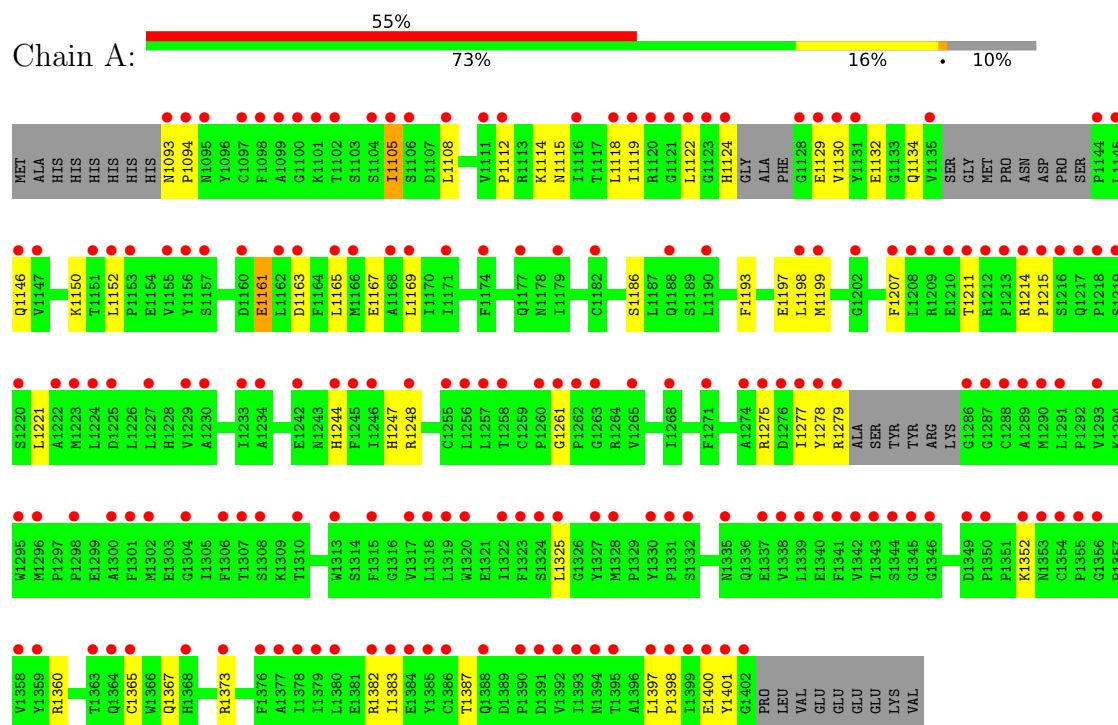
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		

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: ALK TYROSINE KINASE RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.75Å 57.59Å 104.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.60 38.64 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.64-1.60) 99.8 (38.64-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.59Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.215 , 0.258 0.292 , 0.322	Depositor DCC
R_{free} test set	1270 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2558	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5P8

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	0.35	1/2386 (0.0%)	0.68	2/3233 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1401	TYR	C-N	-5.77	1.25	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1261	GLY	CA-C-N	5.86	125.72	119.28
1	A	1261	GLY	C-N-CA	5.86	125.72	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2330	0	2302	60	0
2	A	30	0	19	0	0
3	A	198	0	0	5	0
All	All	2558	0	2321	60	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 (60) 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:1197:GLU:HG2	1:A:1199:MET:HE3	1.54	0.90
1:A:1105:ILE:HG12	1:A:1165:LEU:HD21	1.57	0.84
1:A:1119:ILE:HD11	1:A:1134:GLN:HG3	1.61	0.81
1:A:1105:ILE:HD12	1:A:1105:ILE:H	1.46	0.81
1:A:1199:MET:HA	1:A:1199:MET:HE2	1.65	0.79
1:A:1165:LEU:O	1:A:1169:LEU:HD13	1.86	0.75
1:A:1105:ILE:HG13	1:A:1165:LEU:HD11	1.70	0.73
1:A:1105:ILE:CG1	1:A:1165:LEU:HD21	2.19	0.71
1:A:1105:ILE:HD12	1:A:1105:ILE:N	2.07	0.68
1:A:1152:LEU:HD21	1:A:1161:GLU:HG2	1.78	0.65
1:A:1365:CYS:O	1:A:1373:ARG:HD2	1.97	0.65
1:A:1093:ASN:HB2	1:A:1105:ILE:HD13	1.78	0.65
1:A:1105:ILE:H	1:A:1105:ILE:CD1	2.10	0.65
1:A:1150:LYS:HE2	1:A:1167:GLU:OE1	1.98	0.64
1:A:1163:ASP:HA	1:A:1275:ARG:HD3	1.80	0.63
1:A:1367:GLN:HB2	1:A:1373:ARG:HG2	1.79	0.62
1:A:1214:ARG:HG3	1:A:1215:PRO:HD2	1.84	0.60
1:A:1163:ASP:CA	1:A:1275:ARG:HD3	2.31	0.60
1:A:1124:HIS:HB3	1:A:1129:GLU:HA	1.84	0.59
1:A:1248:ARG:CZ	1:A:1277:ILE:HG21	2.33	0.58
1:A:1093:ASN:ND2	1:A:1105:ILE:HD13	2.19	0.58
1:A:1108:LEU:HD11	1:A:1169:LEU:CD1	2.33	0.57
1:A:1093:ASN:HD22	1:A:1105:ILE:HD13	1.68	0.57
1:A:1207:PHE:O	1:A:1211:THR:HG22	2.06	0.56
1:A:1248:ARG:NH1	1:A:1277:ILE:HG21	2.21	0.56
1:A:1382:ARG:HD3	3:A:2177:HOH:O	2.06	0.54
1:A:1383:ILE:O	1:A:1387:THR:HG23	2.08	0.54
1:A:1146:GLN:HG2	1:A:1198:LEU:HD22	1.90	0.53
1:A:1108:LEU:HD11	1:A:1169:LEU:HD12	1.89	0.53
1:A:1244:HIS:HD2	3:A:2006:HOH:O	1.91	0.53
1:A:1211:THR:HG23	1:A:1221:LEU:HD22	1.91	0.52
1:A:1114:LYS:HG3	1:A:1115:ASN:ND2	2.26	0.51
1:A:1279:ARG:HA	1:A:1279:ARG:HE	1.77	0.50
1:A:1124:HIS:HD2	1:A:1130:VAL:H	1.60	0.50
1:A:1124:HIS:CD2	1:A:1129:GLU:HB3	2.47	0.49
1:A:1163:ASP:HB3	1:A:1275:ARG:CZ	2.43	0.48
1:A:1247:HIS:O	1:A:1248:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:LEU:HD21	1:A:1132:GLU:HB2	1.97	0.47
1:A:1352:LYS:HD2	1:A:1398:PRO:CB	2.45	0.47
1:A:1325:LEU:HD21	1:A:1397:LEU:HD22	1.95	0.46
1:A:1119:ILE:HD11	1:A:1134:GLN:CG	2.38	0.45
1:A:1146:GLN:HG2	1:A:1198:LEU:CD2	2.46	0.45
1:A:1352:LYS:HD2	1:A:1398:PRO:HB3	1.99	0.45
1:A:1167:GLU:CD	3:A:2047:HOH:O	2.60	0.44
1:A:1115:ASN:N	1:A:1115:ASN:HD22	2.15	0.44
1:A:1163:ASP:CB	1:A:1275:ARG:HD3	2.48	0.44
1:A:1112:PRO:HG2	1:A:1115:ASN:CG	2.43	0.44
1:A:1279:ARG:HA	1:A:1279:ARG:NE	2.34	0.43
1:A:1118:LEU:HD22	3:A:2002:HOH:O	2.17	0.43
1:A:1186:SER:HB3	1:A:1193:PHE:HB2	2.01	0.43
1:A:1214:ARG:HG3	1:A:1215:PRO:CD	2.47	0.42
1:A:1112:PRO:HG2	1:A:1115:ASN:OD1	2.19	0.42
1:A:1214:ARG:HE	1:A:1400:GLU:HG3	1.85	0.42
1:A:1367:GLN:O	1:A:1373:ARG:HD3	2.19	0.42
1:A:1124:HIS:HB3	1:A:1129:GLU:HG2	2.01	0.41
1:A:1325:LEU:N	1:A:1325:LEU:HD22	2.35	0.41
1:A:1163:ASP:C	1:A:1275:ARG:HH11	2.28	0.41
1:A:1278:TYR:O	1:A:1279:ARG:HB2	2.21	0.40
1:A:1199:MET:HE1	3:A:2068:HOH:O	2.22	0.40
1:A:1093:ASN:HA	1:A:1094:PRO:HD3	1.85	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	288/327 (88%)	283 (98%)	5 (2%)	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	259/285 (91%)	256 (99%)	3 (1%)	63 43

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1105	ILE
1	A	1161	GLU
1	A	1360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1093	ASN
1	A	1115	ASN
1	A	1124	HIS
1	A	1134	GLN
1	A	1188	GLN
1	A	1217	GLN
1	A	1238	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

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	5P8	A	2402	-	31,33,33	2.09	9 (29%)	39,49,49	1.69	8 (20%)

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	5P8	A	2402	-	-	2/24/26/26	0/3/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2402	5P8	C27-N26	5.90	1.44	1.34
2	A	2402	5P8	C11-C10	4.62	1.45	1.40
2	A	2402	5P8	C28-N26	3.15	1.51	1.46
2	A	2402	5P8	C15-C10	3.11	1.44	1.39
2	A	2402	5P8	C2-N17	2.68	1.41	1.34
2	A	2402	5P8	C12-C11	2.67	1.44	1.39
2	A	2402	5P8	C15-C14	2.61	1.42	1.37
2	A	2402	5P8	C6-C1	2.18	1.42	1.38
2	A	2402	5P8	C10-C8	2.11	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2402	5P8	C19-N20-N21	4.03	114.42	111.20
2	A	2402	5P8	C5-C6-C1	3.52	124.32	119.60
2	A	2402	5P8	C6-C5-C4	-3.34	114.49	117.92
2	A	2402	5P8	C4-C5-C18	3.29	125.68	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2402	5P8	O30-C27-C11	-3.13	113.91	120.06
2	A	2402	5P8	C28-C22-N21	-2.76	116.64	119.63
2	A	2402	5P8	C29-N26-C27	-2.59	116.46	123.14
2	A	2402	5P8	C28-N26-C27	2.53	126.58	119.97

There are no chirality outliers.

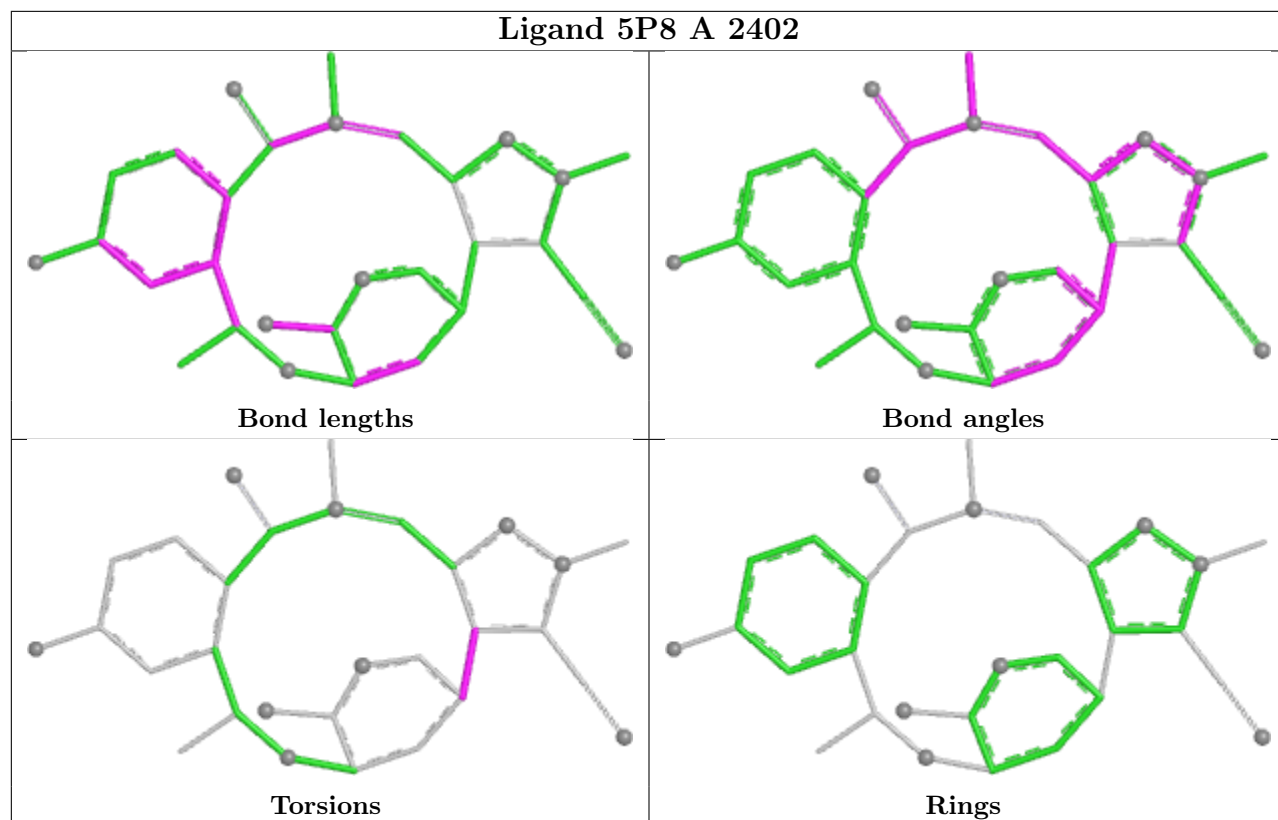
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2402	5P8	C22-C18-C5-C6
2	A	2402	5P8	C19-C18-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

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	293/327 (89%)	2.49	181 (61%) 0 0	11, 29, 61, 77	3 (1%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1277	ILE	6.9
1	A	1218	PRO	5.9
1	A	1105	ILE	5.8
1	A	1101	LYS	5.6
1	A	1123	GLY	5.4
1	A	1124	HIS	5.4
1	A	1288	CYS	5.4
1	A	1165	LEU	5.3
1	A	1155	VAL	5.1
1	A	1211	THR	5.1
1	A	1122	LEU	4.9
1	A	1400	GLU	4.9
1	A	1094	PRO	4.9
1	A	1129	GLU	4.9
1	A	1144	PRO	4.9
1	A	1213	PRO	4.8
1	A	1261	GLY	4.8
1	A	1097[A]	CYS	4.7
1	A	1099	ALA	4.7
1	A	1399	ILE	4.6
1	A	1093	ASN	4.6
1	A	1156	TYR	4.6
1	A	1177	GLN	4.5
1	A	1118	LEU	4.3
1	A	1157	SER	4.2
1	A	1278	TYR	4.1
1	A	1345	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1119	ILE	4.1
1	A	1302	MET	4.1
1	A	1104	SER	4.1
1	A	1319	LEU	4.0
1	A	1385	TYR	4.0
1	A	1100	GLY	4.0
1	A	1219	SER	3.9
1	A	1274	ALA	3.9
1	A	1215	PRO	3.9
1	A	1130	VAL	3.8
1	A	1350	PRO	3.8
1	A	1401	TYR	3.8
1	A	1392	VAL	3.7
1	A	1169	LEU	3.7
1	A	1289	ALA	3.7
1	A	1298	PRO	3.6
1	A	1402	GLY	3.6
1	A	1308	SER	3.6
1	A	1262	PRO	3.6
1	A	1398	PRO	3.6
1	A	1160	ASP	3.6
1	A	1301	PHE	3.5
1	A	1353	ASN	3.5
1	A	1128	GLY	3.5
1	A	1287	GLY	3.5
1	A	1390	PRO	3.5
1	A	1220	SER	3.5
1	A	1394	ASN	3.4
1	A	1325	LEU	3.4
1	A	1384	GLU	3.4
1	A	1121	GLY	3.4
1	A	1304	GLY	3.3
1	A	1339	LEU	3.3
1	A	1286	GLY	3.2
1	A	1346	GLY	3.2
1	A	1217	GLN	3.2
1	A	1102	THR	3.2
1	A	1248	ARG	3.2
1	A	1223	MET	3.2
1	A	1098	PHE	3.2
1	A	1256	LEU	3.2
1	A	1376	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1368	HIS	3.2
1	A	1214	ARG	3.1
1	A	1151	THR	3.1
1	A	1111	VAL	3.1
1	A	1293	VAL	3.1
1	A	1222	ALA	3.1
1	A	1216	SER	3.1
1	A	1355	PRO	3.0
1	A	1257	LEU	3.0
1	A	1095	ASN	3.0
1	A	1359	TYR	3.0
1	A	1244	HIS	3.0
1	A	1382	ARG	3.0
1	A	1343	THR	3.0
1	A	1145	LEU	3.0
1	A	1291	LEU	3.0
1	A	1207	PHE	3.0
1	A	1344	SER	2.9
1	A	1208	LEU	2.9
1	A	1356	GLY	2.9
1	A	1106	SER	2.9
1	A	1341	PHE	2.9
1	A	1146	GLN	2.9
1	A	1364	GLN	2.9
1	A	1162	LEU	2.9
1	A	1246	ILE	2.9
1	A	1234	ALA	2.8
1	A	1152	LEU	2.8
1	A	1373	ARG	2.8
1	A	1363	THR	2.8
1	A	1342	VAL	2.8
1	A	1318	LEU	2.8
1	A	1354	CYS	2.8
1	A	1315	PHE	2.8
1	A	1331	PRO	2.8
1	A	1393	ILE	2.8
1	A	1380	LEU	2.7
1	A	1383	ILE	2.7
1	A	1209	ARG	2.7
1	A	1328	MET	2.7
1	A	1338	VAL	2.7
1	A	1224	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1210	GLU	2.7
1	A	1391	ASP	2.7
1	A	1112	PRO	2.7
1	A	1332	SER	2.7
1	A	1358	VAL	2.6
1	A	1378	ILE	2.6
1	A	1263	GLY	2.6
1	A	1310	THR	2.6
1	A	1198	LEU	2.6
1	A	1386	CYS	2.6
1	A	1260	PRO	2.6
1	A	1202	GLY	2.6
1	A	1255	CYS	2.6
1	A	1327	TYR	2.6
1	A	1306	PHE	2.5
1	A	1279	ARG	2.5
1	A	1379	ILE	2.5
1	A	1300	ALA	2.5
1	A	1295	TRP	2.5
1	A	1324	SER	2.5
1	A	1349	ASP	2.5
1	A	1171	ILE	2.5
1	A	1322	ILE	2.5
1	A	1212	ARG	2.5
1	A	1135	VAL	2.5
1	A	1233	ILE	2.5
1	A	1317	VAL	2.5
1	A	1120	ARG	2.5
1	A	1275	ARG	2.5
1	A	1320	TRP	2.4
1	A	1242	GLU	2.4
1	A	1395	THR	2.4
1	A	1276	ASP	2.4
1	A	1268	ILE	2.4
1	A	1245	PHE	2.3
1	A	1147	VAL	2.3
1	A	1265	VAL	2.3
1	A	1166	MET	2.3
1	A	1230	ALA	2.3
1	A	1227	LEU	2.3
1	A	1397	LEU	2.3
1	A	1258	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1225	ASP	2.2
1	A	1271	PHE	2.2
1	A	1323	PHE	2.2
1	A	1131	TYR	2.2
1	A	1330	TYR	2.2
1	A	1153	PRO	2.2
1	A	1199	MET	2.2
1	A	1365	CYS	2.2
1	A	1340	GLU	2.2
1	A	1108	LEU	2.2
1	A	1174	PHE	2.2
1	A	1179	ILE	2.2
1	A	1296	MET	2.1
1	A	1168	ALA	2.1
1	A	1182	CYS	2.1
1	A	1313	TRP	2.1
1	A	1290	MET	2.1
1	A	1229	VAL	2.1
1	A	1352	LYS	2.1
1	A	1190	LEU	2.1
1	A	1337	GLU	2.1
1	A	1335	ASN	2.0
1	A	1188	GLN	2.0
1	A	1388	GLN	2.0
1	A	1163	ASP	2.0
1	A	1307	THR	2.0
1	A	1116	ILE	2.0
1	A	1377	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.

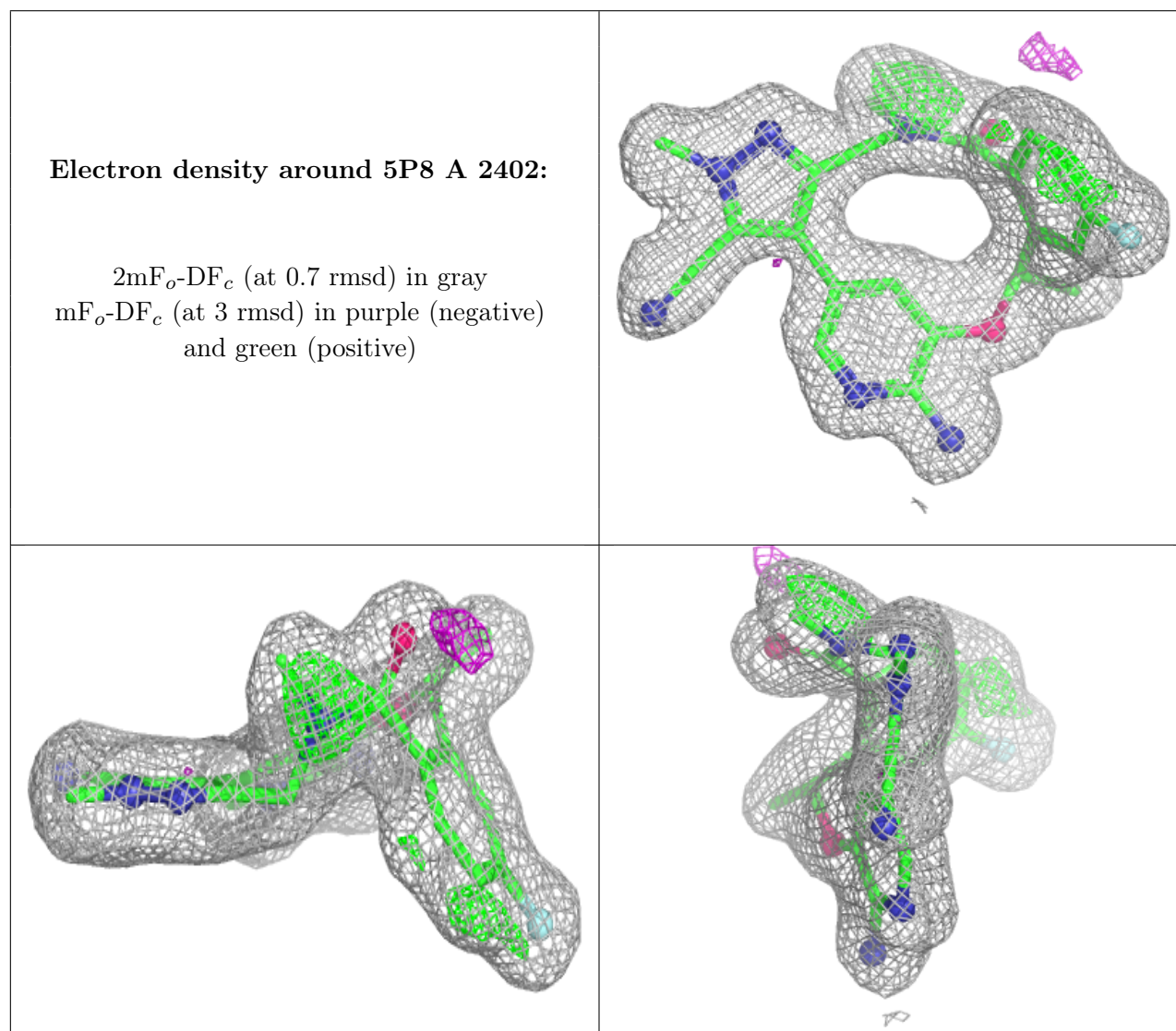
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	5P8	A	2402	30/30	0.85	0.13	23,27,30,31	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.