



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:56 AM UTC

PDB ID : 5AAA / pdb_00005aaa
Title : Structure of L1198F Mutant Human Anaplastic Lymphoma Kinase in Complex with Crizotinib
Authors : McTigue, M.; Deng, Y.; Liu, W.; Brooun, A.; Stewart, A.
Deposited on : 2015-07-23
Resolution : 1.73 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)
Xtrriage (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

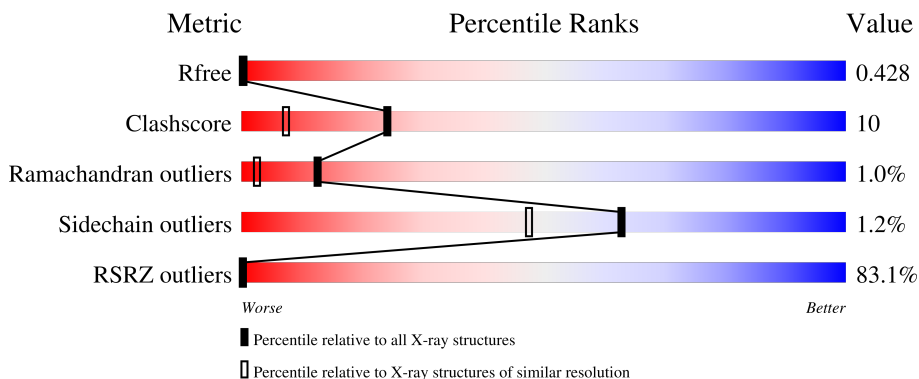
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2607 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.

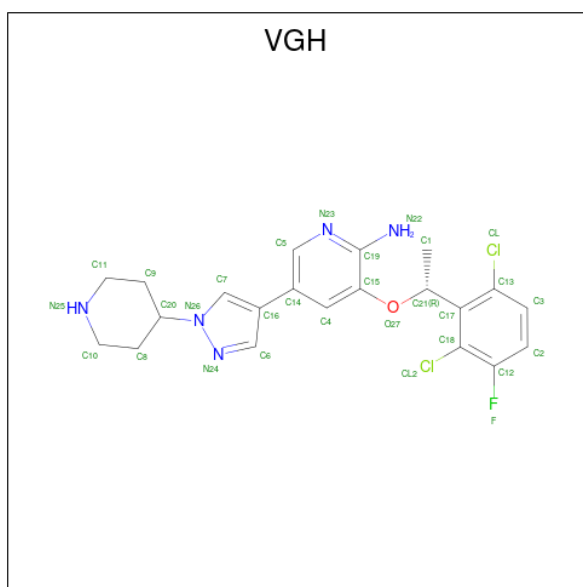
- Molecule 1 is a protein called ALK TYROSINE KINASE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	295	2350	1498	401	428	23	0	4	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	1198	PHE	LEU	engineered mutation	UNP Q9UM73

- Molecule 2 is 3-[(1R)-1-(2,6-dichloro-3-fluorophenyl)ethoxy]-5-(1-piperidin-4-yl-1H-pyrazol-4-yl)pyridin-2-amine (CCD ID: VGH) (formula: C₂₁H₂₂Cl₂FN₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
2	A	1	30	21	2	1	5	1	0	0

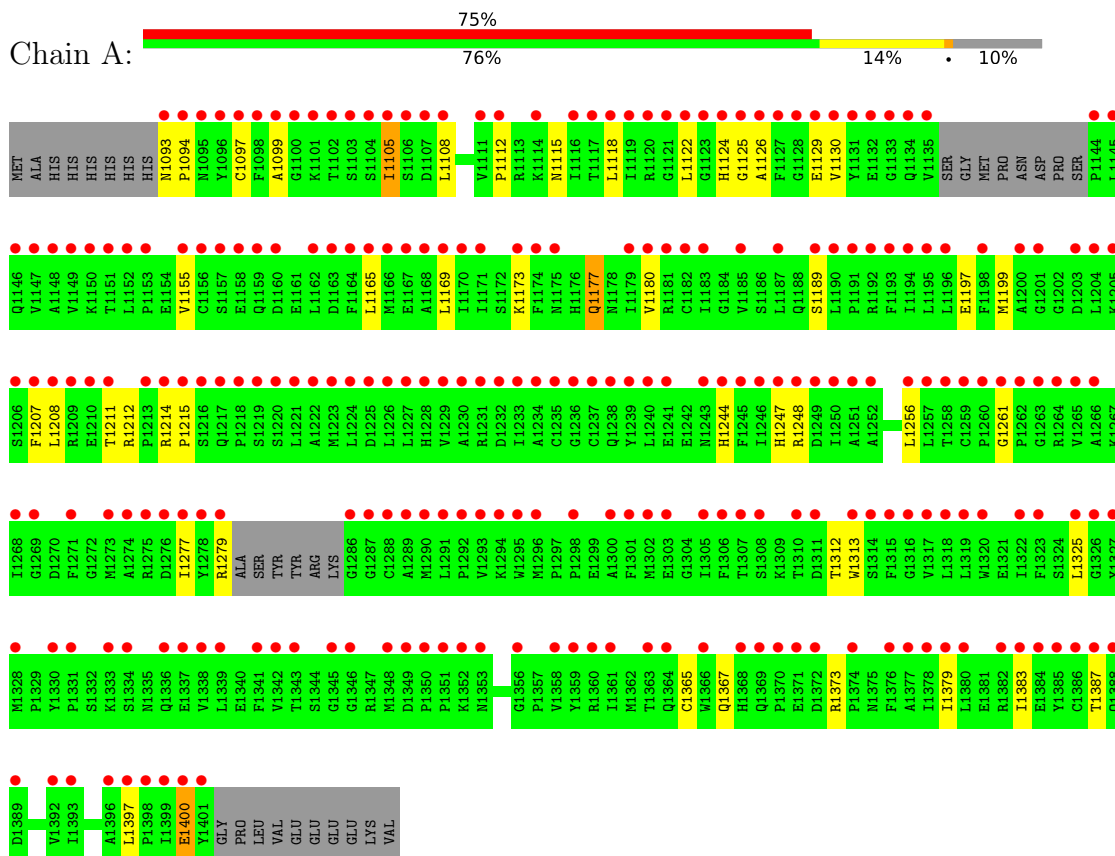
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	227	Total	O	0	0
			227	227		

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	51.47Å 57.28Å 104.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.35 – 1.73 52.35 – 2.02	Depositor EDS
% Data completeness (in resolution range)	89.5 (52.35-1.73) 95.7 (52.35-2.02)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.01Å)	Xtrriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.200 , 0.206 0.420 , 0.428	Depositor DCC
R_{free} test set	591 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtrriage
Anisotropy	0.608	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	2607	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: VGH

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	0.34	1/2408 (0.0%)	0.67	3/3263 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	GLU	C-N	-5.83	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1261	GLY	CA-C-N	7.23	127.23	119.28
1	A	1261	GLY	C-N-CA	7.23	127.23	119.28
1	A	1099	ALA	CB-CA-C	-5.20	110.60	116.63

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	2350	0	2317	46	0
2	A	30	0	22	3	0
3	A	227	0	0	4	0
All	All	2607	0	2339	47	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 10.

All (47) 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:1105:ILE:HD12	1:A:1105:ILE:H	1.20	1.03
1:A:1124:HIS:HB3	1:A:1129:GLU:HA	1.56	0.87
1:A:1199:MET:HA	1:A:1199:MET:HE2	1.60	0.83
1:A:1197:GLU:HG2	1:A:1199:MET:HE3	1.60	0.81
1:A:1105:ILE:HG13	1:A:1165:LEU:HD11	1.61	0.81
1:A:1105:ILE:H	1:A:1105:ILE:CD1	1.94	0.81
1:A:1105:ILE:HD12	1:A:1105:ILE:N	2.00	0.75
1:A:1093:ASN:HB2	1:A:1105:ILE:HD13	1.69	0.74
1:A:1214:ARG:HG3	1:A:1215:PRO:HD2	1.69	0.74
1:A:1165:LEU:O	1:A:1169:LEU:HD13	1.95	0.66
1:A:1248:ARG:CZ	1:A:1277:ILE:HG21	2.25	0.65
1:A:1279:ARG:HA	1:A:1279:ARG:HE	1.60	0.65
1:A:1367:GLN:O	1:A:1373:ARG:HD3	1.98	0.63
1:A:1093:ASN:HB2	1:A:1105:ILE:CD1	2.29	0.62
1:A:1097[A]:CYS:HB3	3:A:2029:HOH:O	2.00	0.62
1:A:1155:VAL:O	1:A:1155:VAL:HG23	2.02	0.59
1:A:1367:GLN:HB2	1:A:1373:ARG:HG2	1.85	0.58
1:A:1244:HIS:HD2	3:A:2008:HOH:O	1.86	0.58
1:A:1279:ARG:HA	1:A:1279:ARG:NE	2.19	0.57
1:A:1248:ARG:NH1	1:A:1277:ILE:HG21	2.20	0.57
1:A:1177:GLN:H	1:A:1177:GLN:NE2	2.03	0.57
1:A:1105:ILE:HG13	1:A:1165:LEU:CD1	2.32	0.55
1:A:1112:PRO:HG2	1:A:1115:ASN:OD1	2.06	0.55
1:A:1180:VAL:HG21	1:A:1256:LEU:HD12	1.89	0.55
1:A:1097[B]:CYS:HB2	3:A:2029:HOH:O	2.07	0.54
1:A:1208:LEU:O	1:A:1212:ARG:HG3	2.08	0.54
1:A:1365:CYS:O	1:A:1373:ARG:HD2	2.07	0.53
1:A:1093:ASN:HD22	1:A:1105:ILE:HD13	1.75	0.52
1:A:1256:LEU:HD11	2:A:9000:VGH:CL2	2.50	0.49
1:A:1108:LEU:HD11	1:A:1169:LEU:CD1	2.43	0.48
1:A:1247:HIS:O	1:A:1248:ARG:HB2	2.14	0.47
2:A:9000:VGH:CL2	2:A:9000:VGH:H12C	2.52	0.47
1:A:1207:PHE:O	1:A:1211:THR:HG22	2.16	0.46
1:A:1124:HIS:CD2	1:A:1129:GLU:HB3	2.51	0.45
1:A:1383:ILE:O	1:A:1387:THR:HG23	2.18	0.43
1:A:1325:LEU:N	1:A:1325:LEU:HD22	2.34	0.42
1:A:1180:VAL:HG13	1:A:1197:GLU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:MET:O	2:A:9000:VGH:H5	2.20	0.41
1:A:1093:ASN:HA	1:A:1094:PRO:HD3	1.84	0.41
1:A:1169:LEU:O	1:A:1173:LYS:HG2	2.20	0.41
1:A:1189:SER:N	3:A:2037:HOH:O	2.50	0.41
1:A:1214:ARG:HG3	1:A:1215:PRO:CD	2.46	0.41
1:A:1313:TRP:CD1	1:A:1313:TRP:C	2.98	0.41
1:A:1122:LEU:HD12	1:A:1130:VAL:HG12	2.03	0.41
1:A:1108:LEU:HD21	1:A:1169:LEU:HD12	2.02	0.41
1:A:1312:THR:HG23	1:A:1379:ILE:HD11	2.03	0.41
1:A:1325:LEU:HD21	1:A:1397:LEU:HD22	2.01	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	293/327 (90%)	281 (96%)	9 (3%)	3 (1%)	12 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1126	ALA
1	A	1400	GLU
1	A	1125	GLY

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	260/285 (91%)	257 (99%)	3 (1%)	63 47

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

Mol	Chain	Res	Type
1	A	1105	ILE
1	A	1118	LEU
1	A	1177	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1093	ASN
1	A	1115	ASN
1	A	1124	HIS
1	A	1177	GLN
1	A	1188	GLN
1	A	1217	GLN
1	A	1238	GLN
1	A	1243	ASN

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](#)

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	VGH	A	9000	-	33,33,33	2.40	16 (48%)	40,47,47	2.22	7 (17%)

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	VGH	A	9000	-	-	0/16/24/24	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9000	VGH	C13-C17	4.90	1.46	1.39
2	A	9000	VGH	C18-C17	4.80	1.47	1.39
2	A	9000	VGH	C18-C12	4.22	1.44	1.38
2	A	9000	VGH	C7-N26	3.93	1.41	1.34
2	A	9000	VGH	N26-N24	-3.86	1.29	1.36
2	A	9000	VGH	C4-C15	3.41	1.44	1.38
2	A	9000	VGH	C19-N22	2.92	1.41	1.34
2	A	9000	VGH	C4-C14	2.75	1.43	1.39
2	A	9000	VGH	C5-C14	2.67	1.43	1.39
2	A	9000	VGH	C6-N24	-2.65	1.29	1.32
2	A	9000	VGH	C6-C16	2.59	1.46	1.40
2	A	9000	VGH	C2-C3	2.26	1.42	1.38
2	A	9000	VGH	C2-C12	2.26	1.42	1.37
2	A	9000	VGH	C14-C16	2.20	1.52	1.48
2	A	9000	VGH	C3-C13	2.09	1.43	1.38
2	A	9000	VGH	O27-C15	2.05	1.41	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9000	VGH	C6-N24-N26	11.11	109.85	104.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9000	VGH	C16-C7-N26	-3.53	104.04	106.82
2	A	9000	VGH	C15-O27-C21	2.82	126.12	119.40
2	A	9000	VGH	C13-C17-C18	2.81	118.09	114.93
2	A	9000	VGH	C17-C13-CL	2.45	123.46	120.54
2	A	9000	VGH	C17-C18-CL2	2.30	123.06	120.37
2	A	9000	VGH	C15-C19-N23	2.04	124.28	121.81

There are no chirality outliers.

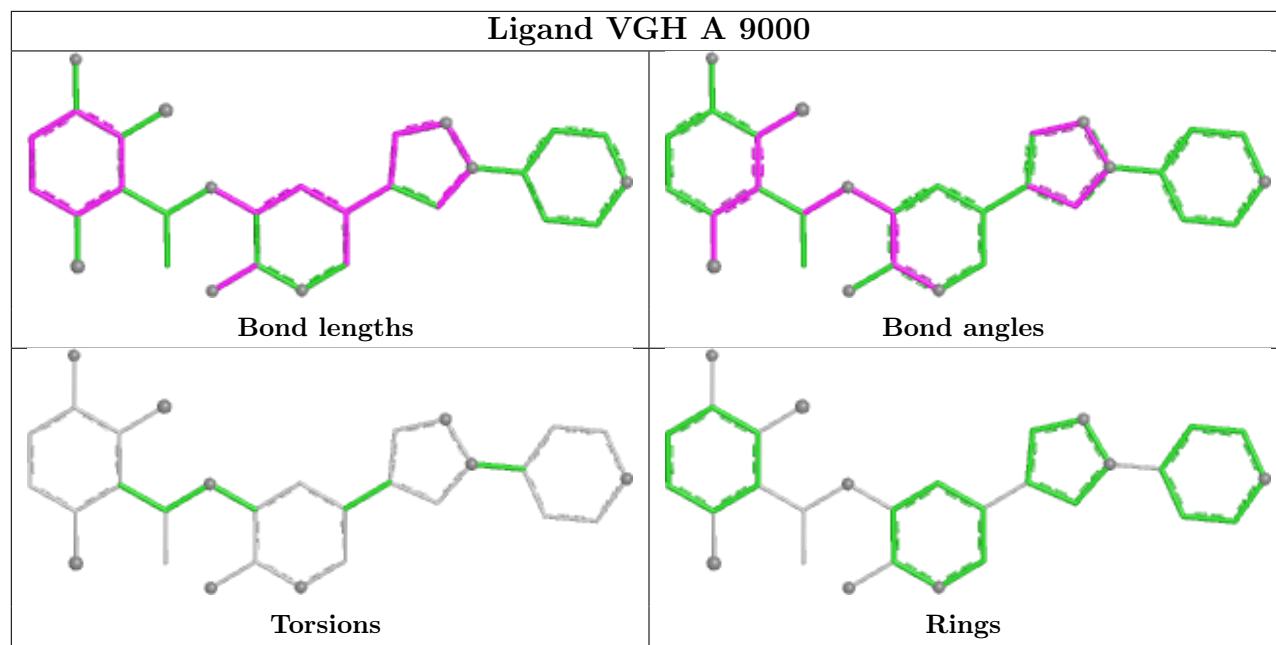
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9000	VGH	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/327 (90%)	3.41	245 (83%) 0 0	9, 26, 56, 72	4 (1%)

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1105	ILE	12.6
1	A	1169	LEU	8.6
1	A	1399	ILE	8.3
1	A	1278	TYR	8.2
1	A	1094	PRO	8.1
1	A	1274	ALA	7.8
1	A	1215	PRO	7.8
1	A	1096[A]	TYR	7.2
1	A	1102	THR	7.1
1	A	1127	PHE	7.0
1	A	1144	PRO	6.8
1	A	1401	TYR	6.8
1	A	1256	LEU	6.7
1	A	1098	PHE	6.7
1	A	1326	GLY	6.6
1	A	1286	GLY	6.6
1	A	1339	LEU	6.5
1	A	1165	LEU	6.4
1	A	1211	THR	6.3
1	A	1122	LEU	6.3
1	A	1097[A]	CYS	6.2
1	A	1155	VAL	6.0
1	A	1273	MET	6.0
1	A	1193	PHE	5.9
1	A	1271	PHE	5.8
1	A	1325	LEU	5.6
1	A	1187	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	1287	GLY	5.6
1	A	1322	ILE	5.6
1	A	1164	PHE	5.5
1	A	1317	VAL	5.4
1	A	1145	LEU	5.4
1	A	1213	PRO	5.4
1	A	1327	TYR	5.4
1	A	1323	PHE	5.3
1	A	1279	ARG	5.3
1	A	1385	TYR	5.2
1	A	1258	THR	5.2
1	A	1168	ALA	5.0
1	A	1131	TYR	5.0
1	A	1320	TRP	4.9
1	A	1307	THR	4.9
1	A	1374	PRO	4.9
1	A	1121	GLY	4.8
1	A	1183	ILE	4.8
1	A	1207	PHE	4.8
1	A	1358	VAL	4.8
1	A	1221	LEU	4.8
1	A	1125	GLY	4.7
1	A	1328	MET	4.7
1	A	1162	LEU	4.7
1	A	1095	ASN	4.7
1	A	1218	PRO	4.7
1	A	1126	ALA	4.7
1	A	1314	SER	4.6
1	A	1376	PHE	4.6
1	A	1180	VAL	4.6
1	A	1301	PHE	4.6
1	A	1100	GLY	4.6
1	A	1238	GLN	4.5
1	A	1263	GLY	4.5
1	A	1400	GLU	4.5
1	A	1369	GLN	4.4
1	A	1190	LEU	4.4
1	A	1302	MET	4.4
1	A	1289	ALA	4.4
1	A	1171	ILE	4.4
1	A	1101	LYS	4.4
1	A	1219	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1333	LYS	4.3
1	A	1359	TYR	4.3
1	A	1341	PHE	4.3
1	A	1342	VAL	4.3
1	A	1265	VAL	4.3
1	A	1247	HIS	4.3
1	A	1363	THR	4.2
1	A	1268	ILE	4.2
1	A	1319	LEU	4.2
1	A	1174	PHE	4.2
1	A	1262	PRO	4.2
1	A	1233	ILE	4.1
1	A	1191	PRO	4.1
1	A	1208	LEU	4.1
1	A	1111	VAL	4.1
1	A	1149	VAL	4.0
1	A	1393	ILE	4.0
1	A	1216	SER	4.0
1	A	1103	SER	4.0
1	A	1346	GLY	4.0
1	A	1194	ILE	3.9
1	A	1296	MET	3.9
1	A	1386	CYS	3.9
1	A	1277	ILE	3.9
1	A	1120	ARG	3.9
1	A	1261	GLY	3.9
1	A	1288	CYS	3.9
1	A	1293	VAL	3.8
1	A	1353	ASN	3.8
1	A	1379	ILE	3.8
1	A	1167	GLU	3.8
1	A	1350	PRO	3.7
1	A	1220	SER	3.7
1	A	1351	PRO	3.6
1	A	1370	PRO	3.6
1	A	1224	LEU	3.6
1	A	1250	ILE	3.6
1	A	1298	PRO	3.6
1	A	1266	ALA	3.6
1	A	1257	LEU	3.6
1	A	1217	GLN	3.6
1	A	1336	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1170	ILE	3.6
1	A	1378	ILE	3.6
1	A	1306	PHE	3.5
1	A	1291	LEU	3.5
1	A	1124	HIS	3.5
1	A	1303	GLU	3.5
1	A	1179	ILE	3.5
1	A	1234	ALA	3.5
1	A	1135	VAL	3.5
1	A	1201	GLY	3.5
1	A	1119	ILE	3.4
1	A	1315	PHE	3.4
1	A	1226	LEU	3.4
1	A	1380	LEU	3.4
1	A	1397	LEU	3.4
1	A	1195	LEU	3.4
1	A	1245	PHE	3.4
1	A	1337	GLU	3.3
1	A	1392	VAL	3.3
1	A	1276	ASP	3.3
1	A	1361	ILE	3.3
1	A	1331	PRO	3.3
1	A	1214	ARG	3.3
1	A	1230	ALA	3.3
1	A	1396	ALA	3.3
1	A	1093	ASN	3.3
1	A	1112	PRO	3.2
1	A	1246	ILE	3.2
1	A	1260	PRO	3.2
1	A	1152	LEU	3.2
1	A	1243	ASN	3.2
1	A	1229	VAL	3.2
1	A	1225	ASP	3.2
1	A	1310	THR	3.2
1	A	1368	HIS	3.1
1	A	1099	ALA	3.1
1	A	1150	LYS	3.1
1	A	1157	SER	3.1
1	A	1116	ILE	3.1
1	A	1237	CYS	3.1
1	A	1114	LYS	3.1
1	A	1185	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1227	LEU	3.1
1	A	1313	TRP	3.0
1	A	1133	GLY	3.0
1	A	1348	MET	3.0
1	A	1196	LEU	3.0
1	A	1203	ASP	3.0
1	A	1308	SER	3.0
1	A	1252	ALA	3.0
1	A	1134	GLN	3.0
1	A	1123	GLY	3.0
1	A	1146	GLN	3.0
1	A	1248	ARG	3.0
1	A	1318	LEU	3.0
1	A	1383	ILE	3.0
1	A	1352	LYS	3.0
1	A	1316	GLY	3.0
1	A	1118	LEU	2.9
1	A	1360	ARG	2.9
1	A	1349	ASP	2.9
1	A	1173	LYS	2.9
1	A	1364[A]	GLN	2.9
1	A	1382	ARG	2.9
1	A	1294	LYS	2.9
1	A	1107	ASP	2.8
1	A	1166	MET	2.8
1	A	1356	GLY	2.8
1	A	1292	PRO	2.8
1	A	1398	PRO	2.8
1	A	1372	ASP	2.8
1	A	1300	ALA	2.7
1	A	1108	LEU	2.7
1	A	1239	TYR	2.7
1	A	1204	LEU	2.7
1	A	1330	TYR	2.7
1	A	1251	ALA	2.7
1	A	1371	GLU	2.6
1	A	1366	TRP	2.6
1	A	1117	THR	2.6
1	A	1235[A]	CYS	2.6
1	A	1345	GLY	2.6
1	A	1198	PHE	2.6
1	A	1156	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1240	LEU	2.6
1	A	1269	GLY	2.5
1	A	1175	ASN	2.5
1	A	1192	ARG	2.5
1	A	1148	ALA	2.5
1	A	1200	ALA	2.5
1	A	1338	VAL	2.5
1	A	1377	ALA	2.5
1	A	1384	GLU	2.5
1	A	1106	SER	2.5
1	A	1206	SER	2.5
1	A	1182	CYS	2.5
1	A	1295	TRP	2.4
1	A	1147	VAL	2.4
1	A	1334	SER	2.4
1	A	1159	GLN	2.4
1	A	1388	GLN	2.4
1	A	1231	ARG	2.4
1	A	1189	SER	2.4
1	A	1209	ARG	2.4
1	A	1244	HIS	2.4
1	A	1153	PRO	2.4
1	A	1160	ASP	2.4
1	A	1275	ARG	2.4
1	A	1228	HIS	2.3
1	A	1132	GLU	2.3
1	A	1130	VAL	2.3
1	A	1222	ALA	2.3
1	A	1104	SER	2.3
1	A	1249	ASP	2.3
1	A	1305	ILE	2.3
1	A	1387	THR	2.2
1	A	1151	THR	2.2
1	A	1223	MET	2.2
1	A	1264	ARG	2.2
1	A	1343	THR	2.2
1	A	1389	ASP	2.2
1	A	1128	GLY	2.2
1	A	1181	ARG	2.2
1	A	1163	ASP	2.1
1	A	1205	LYS	2.1
1	A	1311	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1158	GLU	2.1
1	A	1241	GLU	2.1
1	A	1290	MET	2.1
1	A	1236	GLY	2.1
1	A	1129	GLU	2.1
1	A	1210	GLU	2.1
1	A	1232	ASP	2.0
1	A	1259	CYS	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](#)

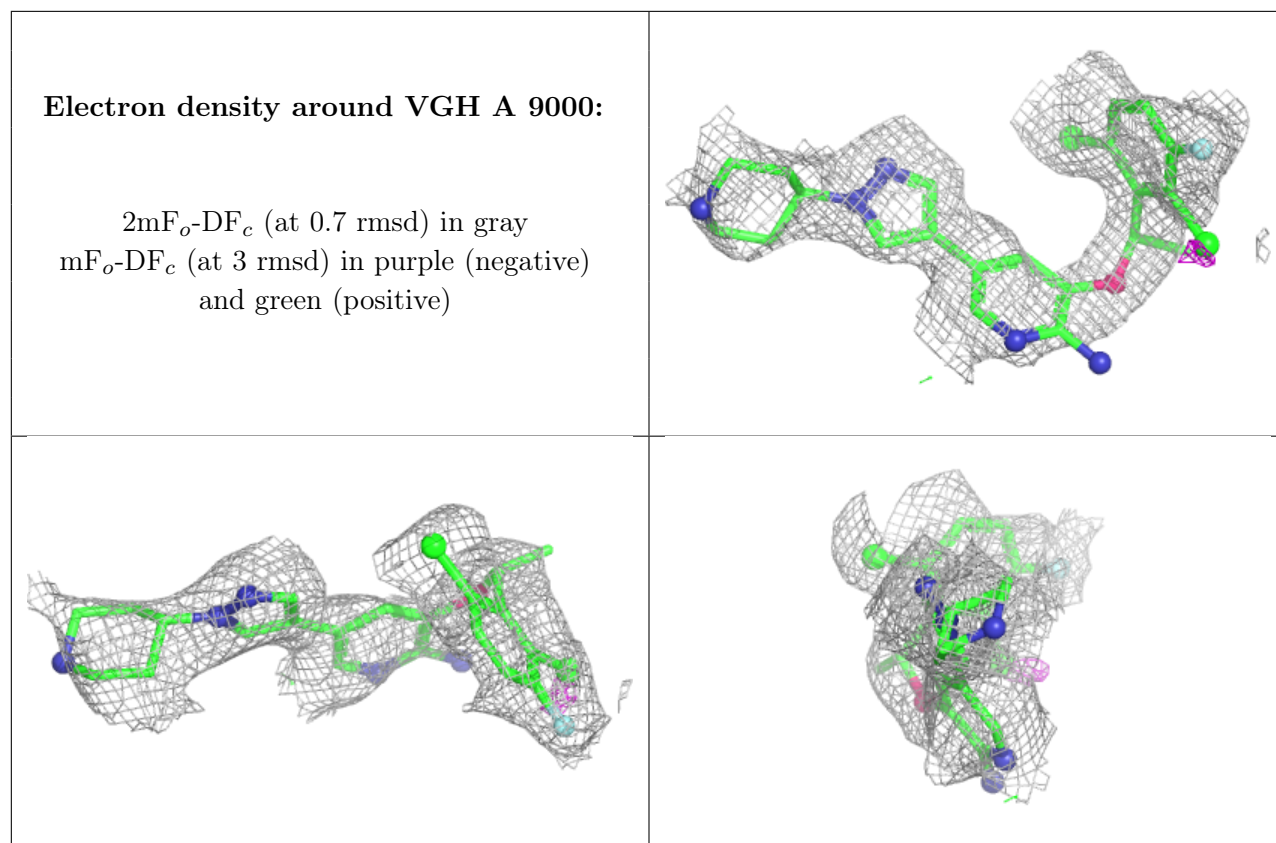
There are no oligosaccharides in this entry.

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	VGH	A	9000	30/30	0.57	0.19	24,33,42,52	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.