



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:10 AM UTC

PDB ID : 3ZBF / pdb_00003zbf
Title : Structure of Human ROS1 Kinase Domain in Complex with Crizotinib
Authors : McTigue, M.; Deng, Y.; Liu, W.; Brooun, A.; Stewart, A.
Deposited on : 2012-11-08
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

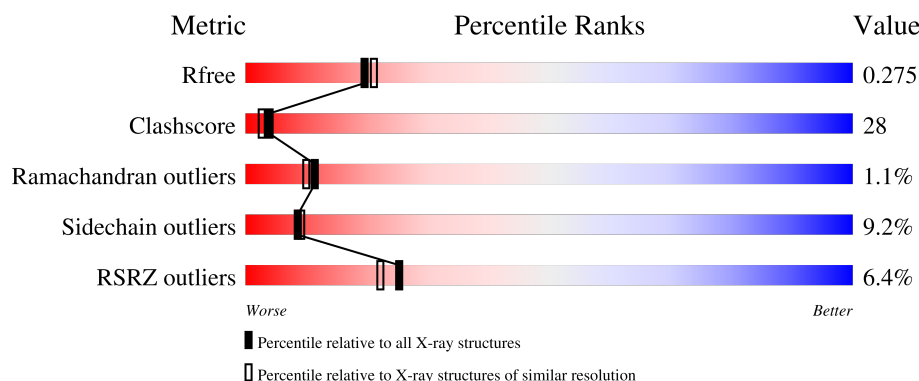
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	322	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2427 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

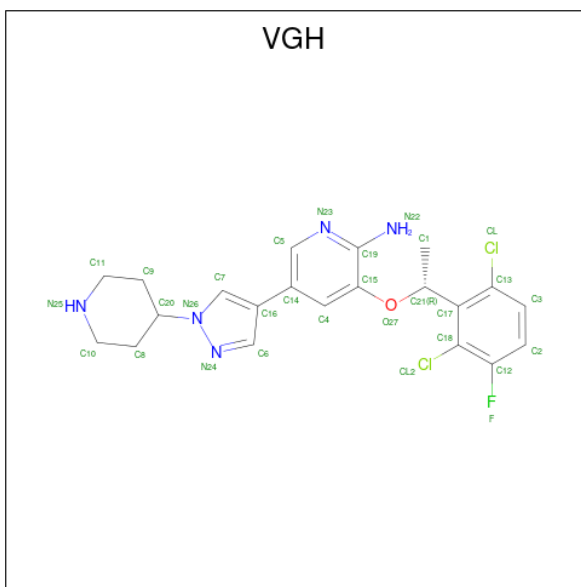
- Molecule 1 is a protein called PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ROS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2260	1457	383	407	13	0	0	1

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1911	MET	-	expression tag	UNP P08922
A	1912	ALA	-	expression tag	UNP P08922
A	1913	HIS	-	expression tag	UNP P08922
A	1914	HIS	-	expression tag	UNP P08922
A	1915	HIS	-	expression tag	UNP P08922
A	1916	HIS	-	expression tag	UNP P08922
A	1917	HIS	-	expression tag	UNP P08922
A	1918	HIS	-	expression tag	UNP P08922
A	1919	ASP	-	expression tag	UNP P08922
A	1920	TYR	-	expression tag	UNP P08922
A	1921	GLY	-	expression tag	UNP P08922
A	1922	ILE	-	expression tag	UNP P08922
A	1923	PRO	-	expression tag	UNP P08922
A	1924	THR	-	expression tag	UNP P08922
A	1925	THR	-	expression tag	UNP P08922
A	1926	GLU	-	expression tag	UNP P08922
A	1927	ASN	-	expression tag	UNP P08922
A	1928	LEU	-	expression tag	UNP P08922
A	1929	TYR	-	expression tag	UNP P08922
A	1930	PHE	-	expression tag	UNP P08922
A	1931	GLN	-	expression tag	UNP P08922
A	1932	GLY	-	expression tag	UNP P08922
A	1933	SER	-	expression tag	UNP P08922

- 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).

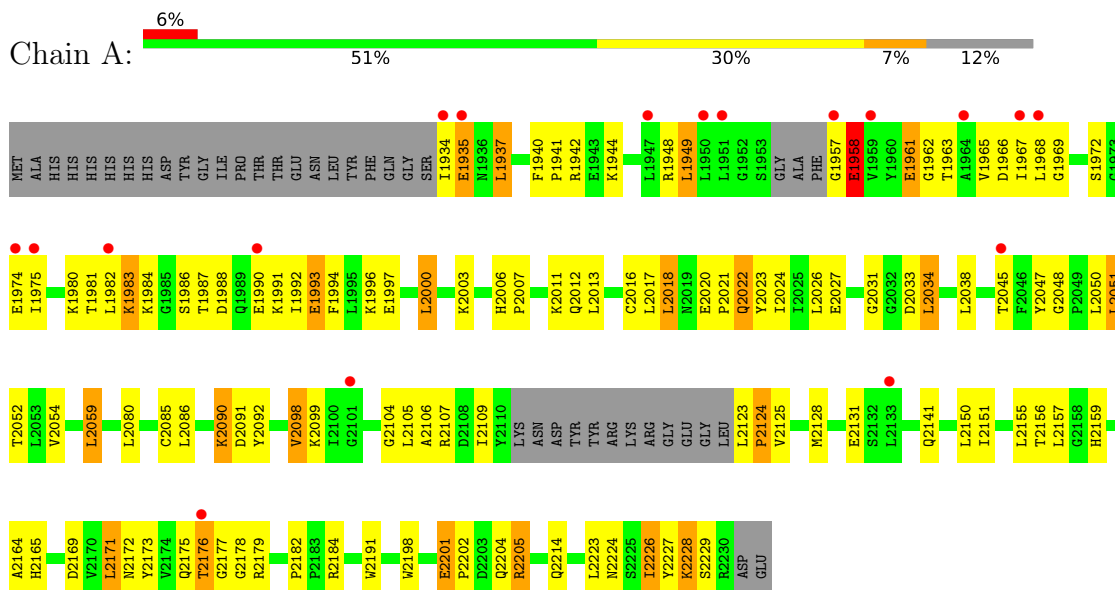


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			30	21	2	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total	O	0	0
			137	137		

- Molecule 1: PROTO-ONCOGENE TYROSINE-PROTEIN KINASE ROS



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	106.85Å 106.85Å 50.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.23 – 2.20 44.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.23-2.20) 97.7 (44.23-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.12Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.233 , 0.282 0.230 , 0.275	Depositor DCC
R_{free} test set	911 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2427	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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	0.40	1/2311 (0.0%)	0.74	4/3133 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2229	SER	C-N	-5.69	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2201	GLU	CA-C-N	5.45	125.79	119.47
1	A	2201	GLU	C-N-CA	5.45	125.79	119.47
1	A	2048	GLY	CA-C-N	5.28	125.22	119.78
1	A	2048	GLY	C-N-CA	5.28	125.22	119.78

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	2260	0	2277	128	0
2	A	30	0	22	2	0
3	A	137	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2427	0	2299	129	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 28.

All (129) 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:1983:LYS:HB2	1:A:1986:SER:HB3	1.32	1.06
1:A:2045:THR:HG22	1:A:2047:TYR:H	1.29	0.97
1:A:1966:ASP:HA	1:A:1972:SER:HB3	1.51	0.90
1:A:2123:LEU:HB3	1:A:2125:VAL:HG13	1.63	0.79
1:A:2151:ILE:O	1:A:2155:LEU:HD23	1.82	0.79
1:A:2224:ASN:O	1:A:2228:LYS:HG3	1.86	0.74
1:A:1991:LYS:HE2	1:A:2022:GLN:HE21	1.55	0.72
1:A:2090:LYS:H	1:A:2090:LYS:CD	2.00	0.71
1:A:1935:GLU:CD	1:A:1935:GLU:H	2.00	0.69
1:A:2156:THR:O	1:A:2159:HIS:HD2	1.75	0.69
1:A:2223:LEU:O	1:A:2226:ILE:HG22	1.93	0.69
1:A:2007:PRO:O	1:A:2099:LYS:HE2	1.93	0.69
1:A:2090:LYS:H	1:A:2090:LYS:HD3	1.58	0.68
1:A:1967:ILE:HB	1:A:1975:ILE:HD11	1.76	0.67
1:A:2226:ILE:C	1:A:2226:ILE:HD13	2.21	0.66
1:A:2179:ARG:NH1	1:A:2198:TRP:O	2.29	0.65
1:A:1983:LYS:HZ2	1:A:1983:LYS:HA	1.60	0.65
1:A:2033:ASP:HA	1:A:2086:LEU:HD23	1.78	0.65
1:A:2018:LEU:H	1:A:2018:LEU:CD2	2.11	0.64
1:A:2123:LEU:N	1:A:2124:PRO:HA	2.13	0.63
1:A:1993:GLU:O	1:A:1996:LYS:HG2	1.97	0.63
1:A:1982:LEU:HD21	1:A:1990:GLU:HG2	1.81	0.63
1:A:1994:PHE:HE2	1:A:2022:GLN:HB2	1.64	0.62
1:A:1993:GLU:O	1:A:1997:GLU:HG3	2.00	0.62
1:A:1957:GLY:O	1:A:1958:GLU:HB2	2.02	0.60
1:A:1948:ARG:NH1	1:A:1949:LEU:HD21	2.17	0.60
1:A:1967:ILE:HG21	1:A:2013:LEU:HB3	1.84	0.60
1:A:1961:GLU:HG3	1:A:1962:GLY:N	2.15	0.59
1:A:1968:LEU:HG	1:A:1975:ILE:HD13	1.86	0.58
1:A:2018:LEU:H	1:A:2018:LEU:HD23	1.68	0.58
1:A:1994:PHE:CE2	1:A:2022:GLN:HB2	2.39	0.58
1:A:2090:LYS:HD3	1:A:2090:LYS:N	2.18	0.58
1:A:2000:LEU:HD22	1:A:2000:LEU:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1988:ASP:O	1:A:1992:ILE:HG12	2.04	0.57
1:A:2123:LEU:HB2	1:A:2125:VAL:H	1.69	0.57
1:A:2182:PRO:HG3	1:A:2191:TRP:CE2	2.39	0.57
1:A:2018:LEU:HD23	3:A:3016:HOH:O	2.03	0.57
1:A:1940:PHE:CE1	1:A:1967:ILE:HG12	2.41	0.56
1:A:2106:ALA:O	1:A:2107:ARG:HD3	2.05	0.56
1:A:2201:GLU:OE2	1:A:2204:GLN:HG3	2.06	0.55
1:A:2202:PRO:HA	1:A:2205:ARG:HD3	1.89	0.55
1:A:1965:VAL:HG12	1:A:1966:ASP:OD2	2.07	0.54
1:A:1984:LYS:HG2	1:A:2020:GLU:HG3	1.89	0.54
1:A:1965:VAL:HG22	1:A:1974:GLU:HG2	1.89	0.54
1:A:1965:VAL:HG22	1:A:1974:GLU:OE2	2.08	0.54
1:A:1942:ARG:NH2	1:A:2021:PRO:O	2.40	0.53
1:A:2016:CYS:HB2	1:A:2023:TYR:HB2	1.89	0.53
1:A:2020:GLU:HG3	1:A:2021:PRO:HA	1.91	0.53
1:A:1991:LYS:HE2	1:A:2022:GLN:NE2	2.21	0.53
1:A:2214:GLN:NE2	3:A:3118:HOH:O	2.42	0.53
1:A:2034:LEU:HD22	1:A:2038:LEU:HG	1.91	0.52
1:A:2011:LYS:HD2	1:A:2027:GLU:CD	2.34	0.52
2:A:3000:VGH:H12C	2:A:3000:VGH:CL2	2.46	0.52
1:A:1993:GLU:HA	1:A:1996:LYS:CD	2.40	0.51
1:A:2175:GLN:C	1:A:2177:GLY:H	2.18	0.51
1:A:1948:ARG:HH11	1:A:1949:LEU:HD21	1.74	0.51
1:A:2124:PRO:O	1:A:2128:MET:HG3	2.10	0.50
1:A:2059:LEU:HD12	1:A:2098:VAL:CG2	2.42	0.50
1:A:1980:LYS:HB3	1:A:2024:ILE:HB	1.94	0.50
1:A:1984:LYS:HG3	1:A:2021:PRO:HG3	1.92	0.50
1:A:2202:PRO:HA	1:A:2205:ARG:NE	2.27	0.49
1:A:1963:THR:OG1	1:A:1974:GLU:HB3	2.12	0.49
1:A:1935:GLU:CD	1:A:1935:GLU:N	2.70	0.49
1:A:2169:ASP:O	1:A:2172:ASN:HB2	2.13	0.49
1:A:2202:PRO:HA	1:A:2205:ARG:CD	2.43	0.49
1:A:1986:SER:HB2	1:A:1990:GLU:OE1	2.13	0.48
1:A:1987:THR:OG1	1:A:1990:GLU:HB2	2.13	0.48
1:A:2003:LYS:HZ2	1:A:2003:LYS:HB3	1.78	0.48
1:A:1994:PHE:CZ	1:A:2024:ILE:HG12	2.48	0.48
1:A:2123:LEU:N	1:A:2124:PRO:CA	2.76	0.48
1:A:2178:GLY:O	1:A:2179:ARG:HD3	2.14	0.48
1:A:2182:PRO:HG3	1:A:2191:TRP:CZ2	2.48	0.48
1:A:2020:GLU:OE2	1:A:2021:PRO:HA	2.14	0.47
1:A:1968:LEU:HD12	1:A:1975:ILE:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2164:ALA:HB3	1:A:2165:HIS:CE1	2.50	0.47
1:A:2171:LEU:O	1:A:2175:GLN:HB2	2.15	0.47
1:A:2045:THR:HG22	1:A:2047:TYR:N	2.13	0.47
1:A:2000:LEU:HD22	1:A:2000:LEU:C	2.40	0.46
1:A:2226:ILE:HG23	1:A:2227:TYR:CD1	2.51	0.46
1:A:1937:LEU:HD23	1:A:2017:LEU:HD11	1.97	0.46
1:A:2179:ARG:HD3	1:A:2179:ARG:HA	1.81	0.46
1:A:2020:GLU:HA	1:A:2021:PRO:C	2.41	0.46
1:A:2184:ARG:H	1:A:2184:ARG:HD3	1.81	0.46
1:A:2090:LYS:HE2	3:A:3037:HOH:O	2.17	0.45
1:A:1982:LEU:HD13	1:A:1982:LEU:C	2.42	0.45
1:A:1993:GLU:HA	1:A:1996:LYS:HG2	1.99	0.45
1:A:1958:GLU:HB3	1:A:1981:THR:OG1	2.16	0.45
1:A:1968:LEU:HG	1:A:1975:ILE:CD1	2.46	0.45
1:A:2150:LEU:HD12	1:A:2150:LEU:O	2.17	0.45
1:A:2018:LEU:HD23	1:A:2018:LEU:N	2.32	0.45
1:A:2086:LEU:HD11	2:A:3000:VGH:CL2	2.54	0.45
1:A:2156:THR:O	1:A:2159:HIS:CD2	2.64	0.45
1:A:2175:GLN:C	1:A:2177:GLY:N	2.75	0.45
1:A:1984:LYS:HG2	1:A:2020:GLU:CG	2.46	0.44
1:A:2182:PRO:HA	1:A:2191:TRP:CZ3	2.52	0.44
1:A:2201:GLU:HA	1:A:2202:PRO:HD3	1.80	0.44
1:A:2226:ILE:HD13	1:A:2226:ILE:O	2.17	0.44
1:A:1941:PRO:HG2	1:A:1944:LYS:HD3	2.00	0.44
1:A:2016:CYS:O	1:A:2022:GLN:HA	2.18	0.44
1:A:2201:GLU:N	1:A:2201:GLU:OE1	2.48	0.44
1:A:2012:GLN:HA	1:A:2026:LEU:HD23	1.99	0.44
1:A:1949:LEU:N	1:A:1949:LEU:HD23	2.32	0.44
1:A:1966:ASP:HA	1:A:1972:SER:CB	2.36	0.43
1:A:1934:ILE:HG23	1:A:1934:ILE:O	2.18	0.43
1:A:2155:LEU:HD22	1:A:2155:LEU:N	2.33	0.43
1:A:2201:GLU:HG2	1:A:2201:GLU:O	2.19	0.43
1:A:2109:ILE:C	1:A:2109:ILE:HD12	2.43	0.42
1:A:2173:TYR:O	1:A:2176:THR:HB	2.20	0.42
1:A:2091:ASP:OD1	1:A:2091:ASP:C	2.62	0.42
1:A:1966:ASP:HB3	1:A:1969:GLY:O	2.20	0.42
1:A:2051:LEU:HD13	1:A:2092:TYR:HD1	1.85	0.42
1:A:1948:ARG:HH22	1:A:1961:GLU:CD	2.28	0.42
1:A:2123:LEU:HD13	1:A:2123:LEU:HA	1.94	0.42
1:A:1982:LEU:HB3	1:A:2022:GLN:HG2	2.01	0.41
1:A:2059:LEU:HD12	1:A:2098:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2020:GLU:CG	1:A:2021:PRO:HA	2.50	0.41
1:A:1982:LEU:HD13	1:A:1983:LYS:N	2.35	0.41
1:A:2104:GLY:O	1:A:2105:LEU:HD12	2.21	0.41
1:A:2034:LEU:HB2	1:A:2085:CYS:HB2	2.02	0.41
1:A:1984:LYS:HB3	1:A:1984:LYS:HE2	1.73	0.41
1:A:2006:HIS:HA	1:A:2007:PRO:HD3	1.96	0.41
1:A:2141:GLN:NE2	1:A:2141:GLN:H	2.18	0.41
1:A:1949:LEU:HG	1:A:1961:GLU:HG2	2.02	0.41
1:A:2176:THR:O	1:A:2176:THR:HG22	2.19	0.41
1:A:1983:LYS:HA	1:A:1983:LYS:NZ	2.31	0.40
1:A:2172:ASN:O	1:A:2175:GLN:HB3	2.20	0.40
1:A:1982:LEU:HD22	1:A:1983:LYS:H	1.85	0.40
1:A:2031:GLY:HA2	1:A:2090:LYS:HA	2.03	0.40
1:A:2052:THR:OG1	1:A:2054:VAL:HG12	2.21	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	276/322 (86%)	265 (96%)	8 (3%)	3 (1%)	11 10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1958	GLU
1	A	2176	THR
1	A	2124	PRO

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	250/284 (88%)	227 (91%)	23 (9%)	8 9

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1935	GLU
1	A	1937	LEU
1	A	1949	LEU
1	A	1958	GLU
1	A	1961	GLU
1	A	1983	LYS
1	A	1993	GLU
1	A	2000	LEU
1	A	2018	LEU
1	A	2022	GLN
1	A	2034	LEU
1	A	2050	LEU
1	A	2051	LEU
1	A	2059	LEU
1	A	2080	LEU
1	A	2090	LYS
1	A	2098	VAL
1	A	2131	GLU
1	A	2157	LEU
1	A	2171	LEU
1	A	2205	ARG
1	A	2226	ILE
1	A	2228	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1989	GLN
1	A	2005	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2022	GLN
1	A	2141	GLN
1	A	2159	HIS
1	A	2185	ASN
1	A	2192	ASN
1	A	2216	GLN
1	A	2224	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3000	-	33,33,33	2.27	13 (39%)	40,47,47	2.21	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	VGH	A	3000	-	-	3/16/24/24	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	VGH	C13-C17	4.74	1.46	1.39
2	A	3000	VGH	C18-C17	4.58	1.47	1.39
2	A	3000	VGH	C18-C12	4.08	1.44	1.38
2	A	3000	VGH	O27-C21	3.78	1.49	1.45
2	A	3000	VGH	N26-N24	-3.41	1.30	1.36
2	A	3000	VGH	C4-C15	2.85	1.43	1.38
2	A	3000	VGH	C19-N22	2.83	1.41	1.34
2	A	3000	VGH	C17-C21	2.62	1.58	1.53
2	A	3000	VGH	C6-C16	2.60	1.46	1.40
2	A	3000	VGH	C5-C14	2.59	1.43	1.39
2	A	3000	VGH	C3-C13	2.21	1.43	1.38
2	A	3000	VGH	C2-C12	2.18	1.42	1.37
2	A	3000	VGH	C4-C14	2.07	1.42	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	VGH	C6-N24-N26	10.04	109.30	104.14
2	A	3000	VGH	C20-N26-C7	-4.09	122.00	128.77
2	A	3000	VGH	C20-N26-N24	3.73	125.50	120.41
2	A	3000	VGH	C17-C18-CL2	2.51	123.31	120.37
2	A	3000	VGH	C17-C13-CL	2.41	123.42	120.54
2	A	3000	VGH	C13-C17-C18	2.35	117.58	114.93
2	A	3000	VGH	C15-O27-C21	2.30	124.87	119.40
2	A	3000	VGH	C16-C7-N26	-2.04	105.22	106.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

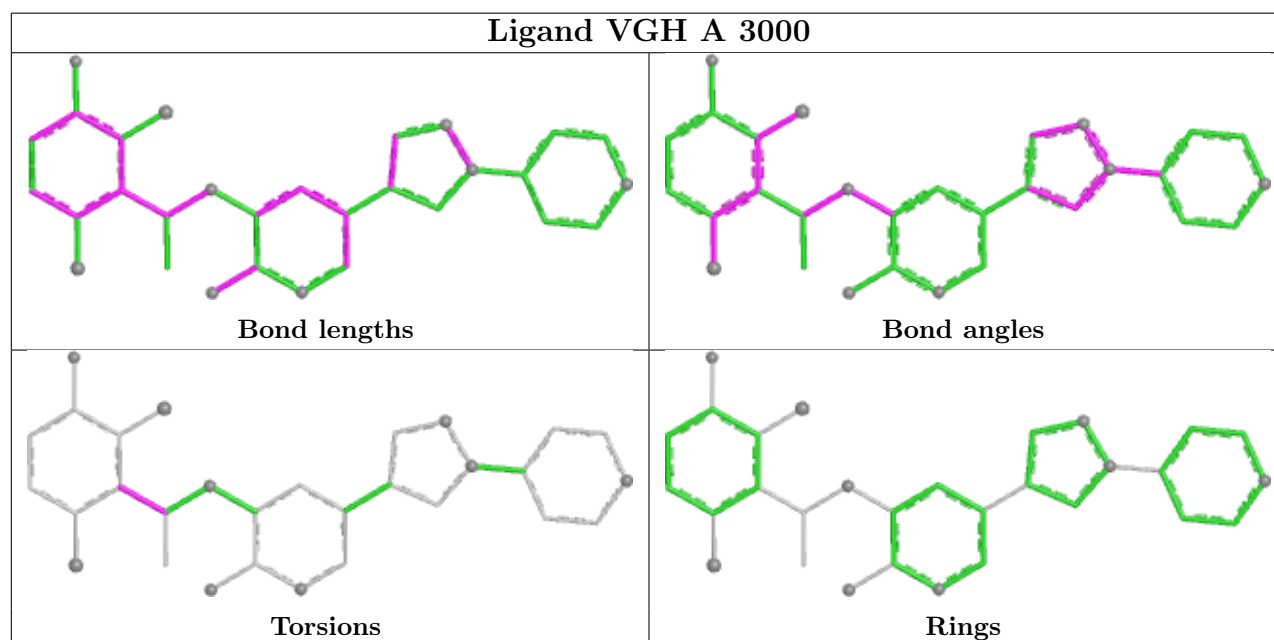
Mol	Chain	Res	Type	Atoms
2	A	3000	VGH	C13-C17-C21-C1
2	A	3000	VGH	C18-C17-C21-C1
2	A	3000	VGH	C13-C17-C21-O27

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3000	VGH	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	282/322 (87%)	0.67	18 (6%)	25 22	27, 50, 88, 99	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1934	ILE	4.1
1	A	2045	THR	3.6
1	A	1967	ILE	3.3
1	A	2101	GLY	3.2
1	A	1935	GLU	3.1
1	A	1959	VAL	3.0
1	A	1964	ALA	2.9
1	A	1968	LEU	2.8
1	A	1990	GLU	2.8
1	A	1947	LEU	2.7
1	A	1957	GLY	2.7
1	A	1951	LEU	2.5
1	A	1950	LEU	2.3
1	A	2176	THR	2.2
1	A	2133	LEU	2.2
1	A	1975	ILE	2.1
1	A	1974	GLU	2.1
1	A	1982	LEU	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](#)

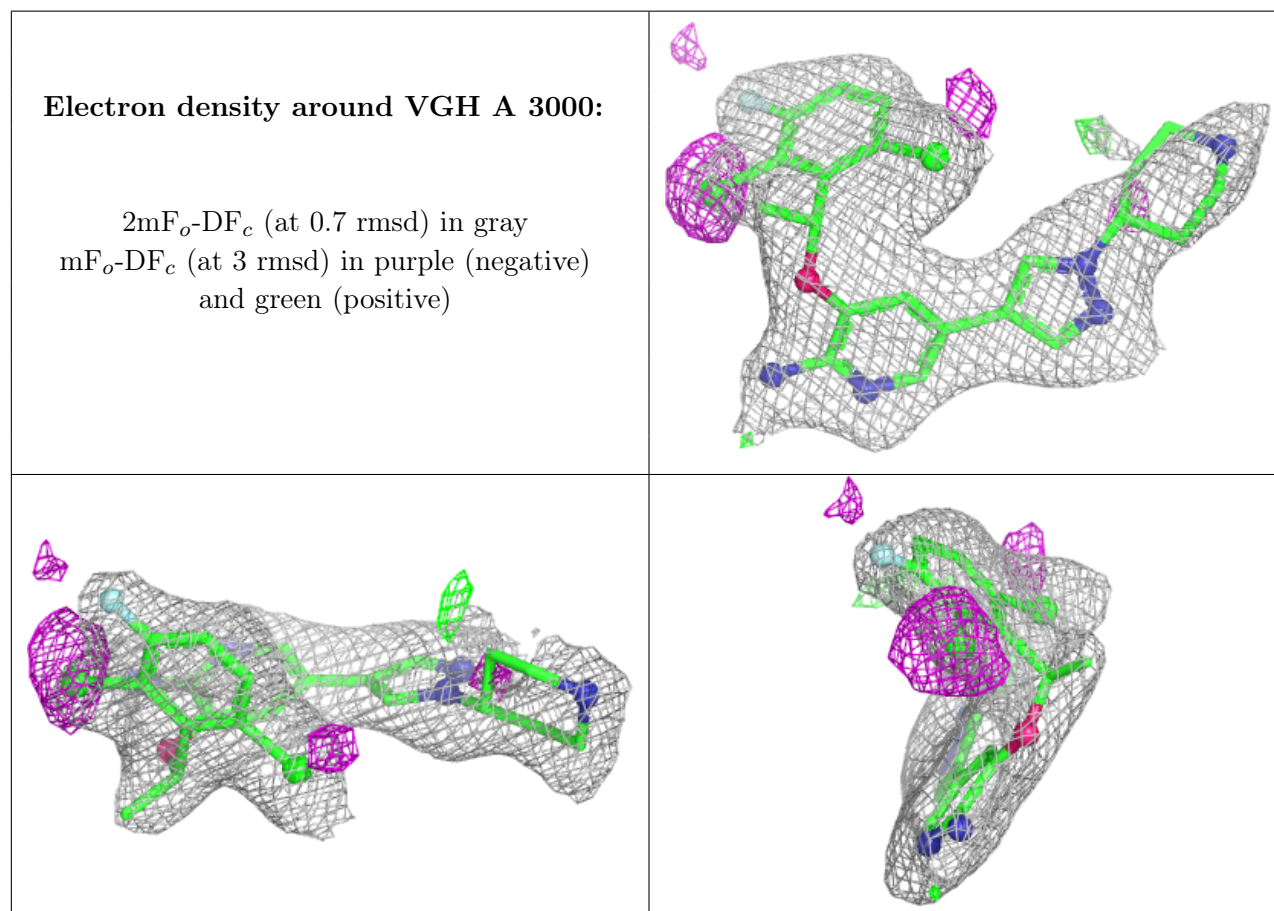
There are no oligosaccharides in this entry.

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	VGH	A	3000	30/30	0.84	0.13	36,51,62,65	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.