

Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 11:43 am GMT

PDB ID : 2UV2

Title : Crystal Structure Of Human Ste20-Like Kinase Bound To 4-(4-(5- Cycloprop

yl-1H-pyrazol-3-ylamino)-quinazolin-2-ylamino)-phenyl)- acetonitrile

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Deposited on : 2007-03-08

Resolution : 2.30 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 (i) 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.36

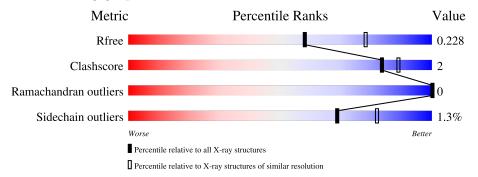


1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 <=5%

Mol	Chain	Length	Quality of chain		
1	Α.	200			
1	A	326	82%	6%	12%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2456 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.

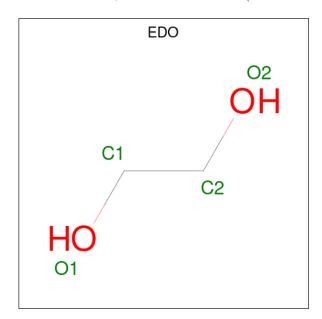
• Molecule 1 is a protein called STE20-LIKE SERINE-THREONINE KINASE.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	A	286	Total 2253	C 1438	N 367	O 436	P 1	S 11	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	THR	LYS	engineered mutation	UNP Q9H2G2
A	183	TPO	THR	microheterogeneity	UNP Q9H2G2

• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

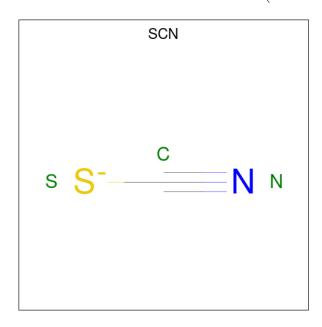
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

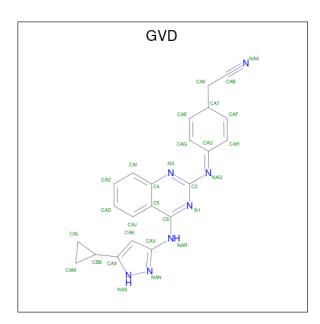
• Molecule 3 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 3		N 1		0	0
3	A	1	Total 3	C 1	N 1	S 1	0	0

• Molecule 4 is [4-({4-[(5-CYCLOPROPYL-1H-PYRAZOL-3-YL)AMINO]QUINAZOLIN-2-YL}IMINO)CYCLOHEXA-2,5-DIEN-1-YL]ACETONITRILE (three-letter code: GVD) (formula: $C_{22}H_{19}N_7$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total 29	C 22	N 7	0	0

• Molecule 5 is water.

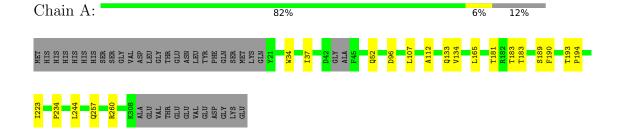
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	148	Total O 148 148	0	0



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. 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. 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: STE20-LIKE SERINE-THREONINE KINASE





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	101.26Å 101.26Å 176.47Å	Donogiton
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 - 2.30	Depositor
Resolution (A)	48.67 - 2.30	EDS
% Data completeness	99.3 (60.00-2.30)	Depositor
(in resolution range)	99.3 (48.67-2.30)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.55 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.198 , 0.234	Depositor
R, R_{free}	0.195 , 0.228	DCC
R_{free} test set	1232 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 42.0	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2456	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: GVD, SCN, TPO, EDO

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).

Mal	Chain	Bond	$\mathbf{lengths}$	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.49	0/2290	0.61	0/3118	

There are no bond length outliers.

There are no bond angle outliers.

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	2253	0	2167	11	0
2	A	20	0	30	3	0
3	A	6	0	0	0	0
4	A	29	0	18	0	0
5	A	148	0	0	1	0
All	All	2456	0	2215	11	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 2.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:A:134:VAL:HG13	2:A:1310:EDO:C2	2.35	0.57
1:A:34:TRP:CD2	1:A:107:LEU:HD22	2.41	0.55
1:A:181:THR:HG21	5:A:2059:HOH:O	2.08	0.52
1:A:133:GLN:HE22	2:A:1313:EDO:H12	1.78	0.47
1:A:223:ILE:HG23	1:A:234:PRO:HD2	1.98	0.45
1:A:190:PHE:CE2	1:A:194:PRO:HG3	2.53	0.44
1:A:257:GLN:OE1	1:A:260:ARG:NH1	2.52	0.43
1:A:112:ALA:HB3	1:A:165:LEU:CG	2.50	0.42
1:A:37:ILE:HD11	1:A:52:GLN:HB2	2.02	0.41
1:A:134:VAL:HG13	2:A:1310:EDO:H21	2.01	0.41
1:A:193:THR:HA	1:A:194:PRO:HD3	1.98	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	Perce	ntiles
1	A	281/326 (86%)	272 (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	Analysed Rotameric		Percentiles	
1	A	$239/288 \ (83\%)$	236 (99%)	3 (1%)	69 82	



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

Mol	Chain	Res	Type
1	A	96	ASP
1	A	189	SER
1	A	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	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)

1 non-standard protein/DNA/RNA residue 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	Mol Type Chain Res		Res	Tiple	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	TPO	A	183[B]	-	8,10,11	1.95	3 (37%)	10,14,16	1.00	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
1	TPO	A	183[B]	-	-	2/9/11/13	-

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
1	A	183[B]	TPO	P-O1P	3.91	1.63	1.50
1	A	183[B]	TPO	P-OG1	2.24	1.63	1.59
1	A	183[B]	TPO	P-O2P	2.05	1.62	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	183[B]	TPO	N-CA-CB-OG1
1	A	183[B]	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	Mol Type Chain Res L		Link	Вс	ond leng	ths	Bond angles			
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	1310	-	3,3,3	0.27	0	2,2,2	0.77	0
2	EDO	A	1309	-	3,3,3	0.50	0	2,2,2	0.38	0
2	EDO	A	1313	-	3,3,3	0.56	0	2,2,2	0.19	0
2	EDO	A	1312	-	3,3,3	0.50	0	2,2,2	0.24	0
3	SCN	A	1314	_	1,2,2	0.27	0	0,1,1	-	-
4	GVD	A	1316	-	28,33,33	2.50	7 (25%)	27,46,46	3.49	8 (29%)
3	SCN	A	1315	-	1,2,2	0.16	0	0,1,1	-	-
2	EDO	A	1311	_	3,3,3	0.43	0	2,2,2	0.47	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
2	EDO	A	1310	-	-	1/1/1/1	-
2	EDO	A	1309	-	-	1/1/1/1	-
2	EDO	A	1313	-	-	1/1/1/1	-
2	EDO	A	1312	-	-	0/1/1/1	-
4	GVD	A	1316	-	-	4/12/27/27	0/5/5/5
2	EDO	A	1311	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
4	A	1316	GVD	NAS-NAN	-6.57	1.23	1.36
4	A	1316	GVD	CAT-CAE	-5.77	1.39	1.50
4	A	1316	GVD	CAT-CAF	-5.45	1.40	1.50
4	A	1316	GVD	CAK-CAV	-4.65	1.34	1.40
4	A	1316	GVD	CAG-CAE	3.36	1.40	1.33
4	A	1316	GVD	CAH-CAF	3.08	1.39	1.33
4	A	1316	GVD	CAV-NAR	-2.13	1.36	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	1316	GVD	CAV-NAN-NAS	13.38	111.78	103.66
4	A	1316	GVD	CAK-CAV-NAN	-6.13	108.01	112.13
4	A	1316	GVD	CAK-CAX-NAS	5.28	110.71	106.16
4	A	1316	GVD	N1-C2-N3	-4.53	121.38	126.91
4	A	1316	GVD	CA0-CAT-CAE	4.35	120.14	111.82
4	A	1316	GVD	CA0-CAT-CAF	4.31	120.07	111.82
4	A	1316	GVD	CA0-CAB-NAA	-2.81	170.42	177.82
4	A	1316	GVD	CBB-CAX-CAK	-2.18	127.49	131.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

\mathbf{M}	ol	Chain	Res	Type	Atoms
4		A	1316	GVD	CAG-CAU-NAQ-C2
4		A	1316	GVD	CAH-CAU-NAQ-C2
4		A	1316	GVD	CAB-CA0-CAT-CAF

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Mol	Chain	Res	Type	Atoms
2	A	1310	EDO	O1-C1-C2-O2
2	A	1309	EDO	O1-C1-C2-O2
2	A	1311	EDO	O1-C1-C2-O2
2	A	1313	EDO	O1-C1-C2-O2
4	A	1316	GVD	CAK-CAX-CBB-CAL

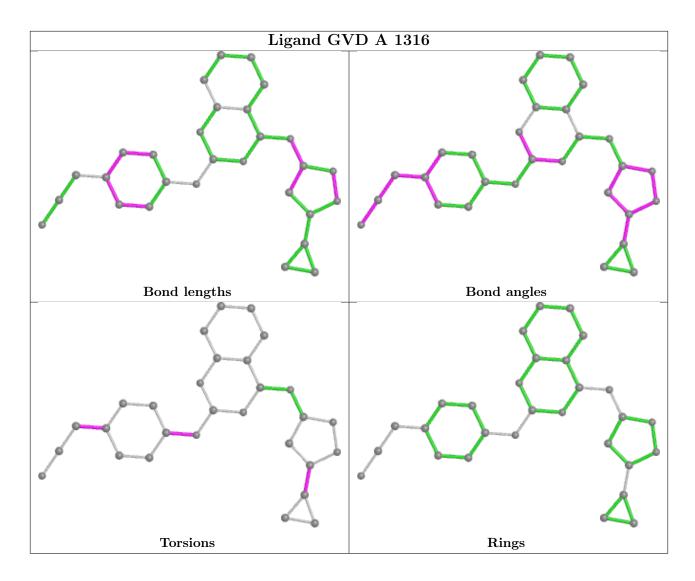
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1310	EDO	2	0
2	A	1313	EDO	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 then 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

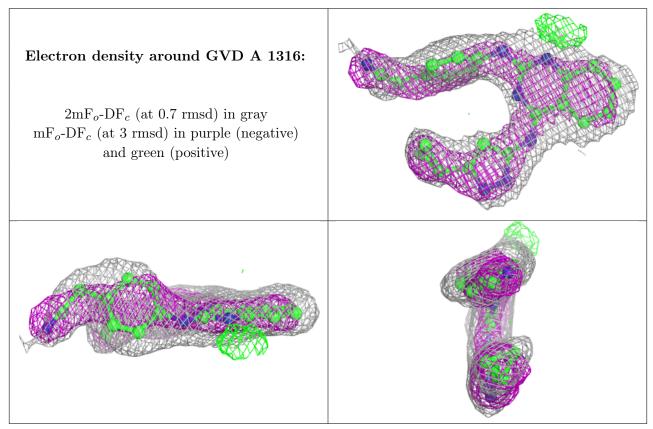
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

