



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7PUE / pdb_00007pue
Title : Human serum and glucocorticoid-regulated kinase 1 in complex with pyrazolopyridine inhibitor 3a
Authors : Dreyer, M.K.; Halland, N.; Nazare, M.
Deposited on : 2021-09-29
Resolution : 2.51 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

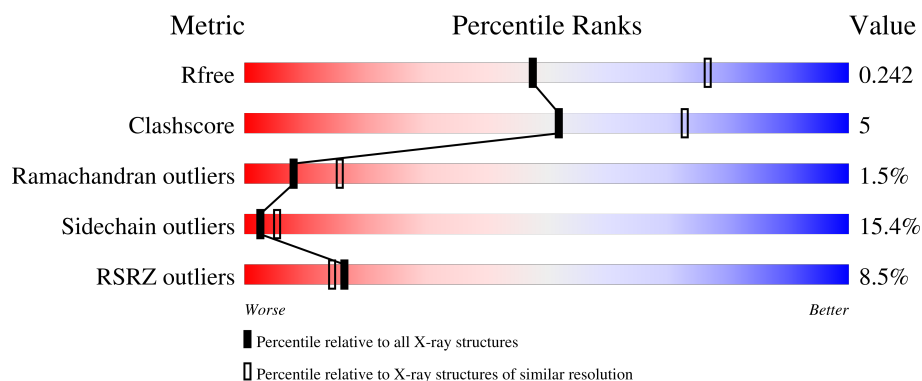
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	375	6% 53% 17% 28%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2226 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.

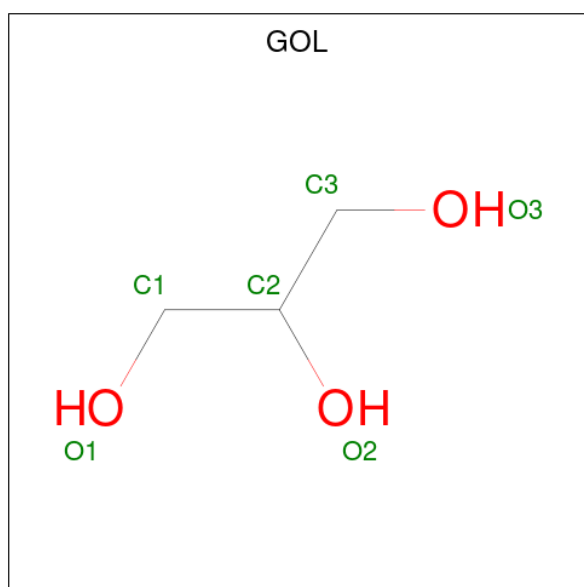
- Molecule 1 is a protein called Serine/threonine-protein kinase Sgk1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	271	2155	1408	363	377	7	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

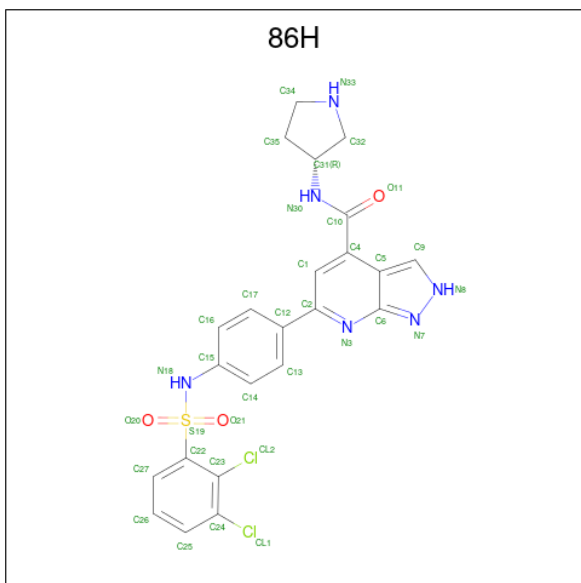
Chain	Residue	Modelled	Actual	Comment	Reference
A	57	GLY	-	expression tag	UNP O00141
A	58	ALA	-	expression tag	UNP O00141
A	59	MET	-	expression tag	UNP O00141
A	192	ALA	ARG	engineered mutation	UNP O00141
A	422	ASP	SER	engineered mutation	UNP O00141

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

- Molecule 3 is 6-[4-[[2,3-bis(chloranyl)phenyl]sulfonylamino]phenyl]- $\{N\}$ -[(3 $\{R\}$)-pyrrolidin-3-yl]-2 $\{H\}$ -pyrazolo[3,4- b]pyridine-4-carboxamide (CCD ID: 86H) (formula: $C_{23}H_{20}Cl_2N_6O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			35	23	2	6	3	1		

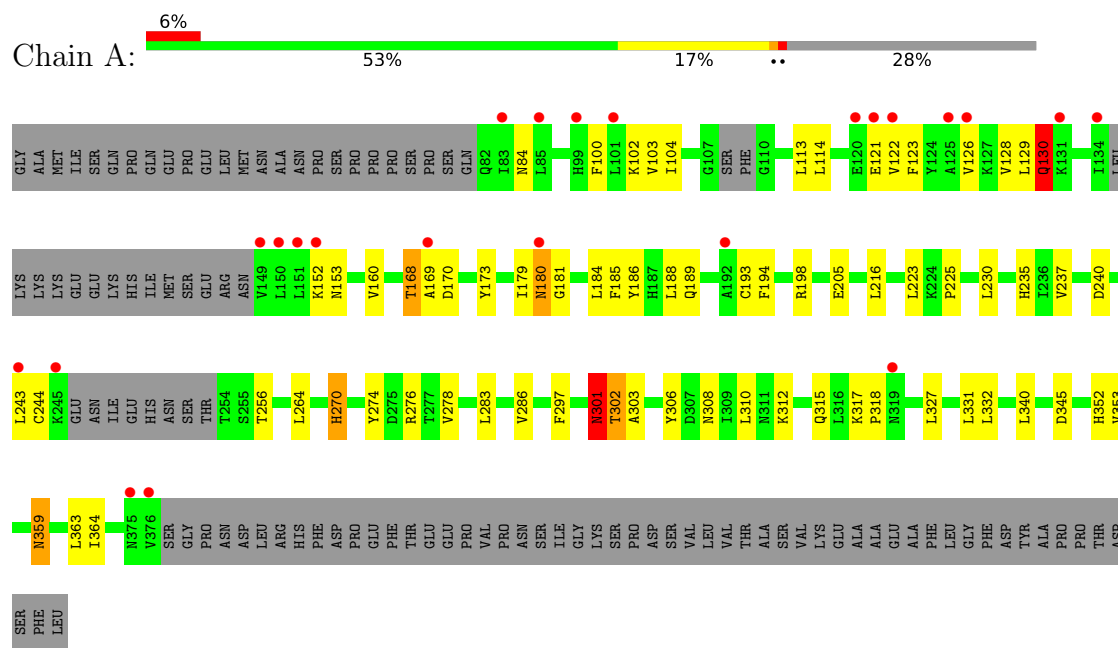
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	24	Total O 24 24	0	0

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: Serine/threonine-protein kinase Sgk1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.44Å 92.44Å 172.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.73 – 2.51 19.73 – 2.51	Depositor EDS
% Data completeness (in resolution range)	70.1 (19.73-2.51) 69.9 (19.73-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.213 , 0.249 0.217 , 0.242	Depositor DCC
R_{free} test set	767 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2226	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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: 86H, GOL

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	0.78	1/2214 (0.0%)	1.22	16/3007 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	ASN	C-N	5.01	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASN	N-CA-C	7.51	119.26	111.14
1	A	318	PRO	N-CA-C	6.72	122.30	114.03
1	A	153	ASN	CA-C-N	6.65	127.91	121.65
1	A	153	ASN	C-N-CA	6.65	127.91	121.65
1	A	153	ASN	N-CA-C	-6.50	106.08	112.97
1	A	179	ILE	CA-C-N	6.11	128.75	120.44
1	A	179	ILE	C-N-CA	6.11	128.75	120.44
1	A	301	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	168	THR	CA-C-N	5.61	132.26	121.54
1	A	168	THR	C-N-CA	5.61	132.26	121.54
1	A	359	ASN	N-CA-C	-5.58	99.42	108.41
1	A	194	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	181	GLY	N-CA-C	5.23	120.42	114.67
1	A	186	TYR	N-CA-C	-5.22	105.67	111.36
1	A	345	ASP	CA-C-N	5.11	127.38	120.38
1	A	345	ASP	C-N-CA	5.11	127.38	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2155	0	2112	22	0
2	A	12	0	16	0	0
3	A	35	0	0	0	0
4	A	24	0	0	1	0
All	All	2226	0	2128	22	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 5.

All (22) 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:270:HIS:CE1	1:A:310:LEU:HD22	2.24	0.72
1:A:129:LEU:O	1:A:130:GLN:HB2	1.93	0.67
1:A:168:THR:HG23	1:A:173:TYR:HE1	1.59	0.66
1:A:205:GLU:OE2	1:A:235:HIS:HD2	1.88	0.57
1:A:301:ASN:HD22	1:A:301:ASN:C	2.13	0.57
1:A:188:LEU:HD11	1:A:193:CYS:HA	1.90	0.54
1:A:274:TYR:HB2	1:A:278:VAL:HG11	1.94	0.49
1:A:100:PHE:HB3	1:A:113:LEU:HD23	1.94	0.48
1:A:274:TYR:HB2	1:A:278:VAL:CG1	2.43	0.48
1:A:185:PHE:CG	1:A:225:PRO:HB3	2.50	0.46
1:A:114:LEU:HD11	1:A:123:PHE:HD2	1.80	0.46
1:A:225:PRO:O	4:A:601:HOH:O	2.21	0.44
1:A:352:HIS:CE1	1:A:353:VAL:HG22	2.53	0.43
1:A:308:ASN:HA	1:A:312:LYS:HB2	2.01	0.43
1:A:327:LEU:HB2	1:A:352:HIS:CE1	2.54	0.42
1:A:168:THR:HG23	1:A:173:TYR:CE1	2.46	0.42
1:A:302:THR:HG22	1:A:306:TYR:CE2	2.54	0.42
1:A:102:LYS:HD3	1:A:104:ILE:HG22	2.00	0.41
1:A:297:PHE:HB3	1:A:308:ASN:HB2	2.02	0.41
1:A:270:HIS:ND1	1:A:310:LEU:HD22	2.35	0.41
1:A:302:THR:HG22	1:A:306:TYR:HE2	1.86	0.41
1:A:301:ASN:HD21	1:A:303:ALA:HB3	1.85	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	263/375 (70%)	232 (88%)	27 (10%)	4 (2%)	8 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	169	ALA
1	A	121	GLU
1	A	170	ASP

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	227/332 (68%)	192 (85%)	35 (15%)	2 5

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	103	VAL
1	A	122	VAL
1	A	126	VAL

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Mol	Chain	Res	Type
1	A	128	VAL
1	A	130	GLN
1	A	152	LYS
1	A	160	VAL
1	A	180	ASN
1	A	184	LEU
1	A	189	GLN
1	A	198	ARG
1	A	216	LEU
1	A	223	LEU
1	A	230	LEU
1	A	237	VAL
1	A	240	ASP
1	A	243	LEU
1	A	244	CYS
1	A	256	THR
1	A	264	LEU
1	A	270	HIS
1	A	276	ARG
1	A	283	LEU
1	A	286	VAL
1	A	301	ASN
1	A	302	THR
1	A	315	GLN
1	A	317	LYS
1	A	331	LEU
1	A	332	LEU
1	A	340	LEU
1	A	359	ASN
1	A	363	LEU
1	A	364	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	82	GLN
1	A	99	HIS
1	A	117	HIS
1	A	153	ASN
1	A	180	ASN
1	A	187	HIS
1	A	189	GLN

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	235	HIS
1	A	301	ASN
1	A	308	ASN
1	A	359	ASN
1	A	365	ASN
1	A	373	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 ⓘ

3 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
2	GOL	A	501	-	5,5,5	0.38	0	5,5,5	0.27	0
3	86H	A	503	-	36,39,39	2.43	7 (19%)	48,57,57	3.80	21 (43%)
2	GOL	A	502	-	5,5,5	0.38	0	5,5,5	0.32	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	GOL	A	501	-	-	2/4/4/4	-
3	86H	A	503	-	-	11/23/30/30	0/5/5/5
2	GOL	A	502	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	86H	C15-N18	-7.00	1.32	1.43
3	A	503	86H	O20-S19	6.41	1.51	1.43
3	A	503	86H	N8-N7	-6.06	1.24	1.36
3	A	503	86H	C12-C2	-5.41	1.40	1.49
3	A	503	86H	O21-S19	4.28	1.48	1.43
3	A	503	86H	C4-C5	-3.80	1.39	1.44
3	A	503	86H	C4-C10	2.98	1.55	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	86H	O21-S19-O20	-14.53	101.87	119.52
3	A	503	86H	C22-S19-N18	12.94	122.54	107.30
3	A	503	86H	C23-C22-S19	-7.34	118.00	123.18
3	A	503	86H	C2-N3-C6	5.47	122.00	117.93
3	A	503	86H	O21-S19-C22	-5.29	98.95	107.68
3	A	503	86H	C5-C6-N3	-5.01	121.04	126.44
3	A	503	86H	C23-C24-CL1	-4.68	116.21	120.51
3	A	503	86H	O20-S19-C22	4.26	114.71	107.68
3	A	503	86H	C24-C23-CL2	-4.25	114.64	120.02
3	A	503	86H	C15-N18-S19	3.84	134.86	122.94
3	A	503	86H	C1-C2-N3	-3.82	117.91	122.34
3	A	503	86H	C27-C22-S19	3.41	122.41	117.51
3	A	503	86H	C25-C24-CL1	2.86	124.06	118.42
3	A	503	86H	C6-N7-N8	2.72	110.13	103.16
3	A	503	86H	O20-S19-N18	2.67	113.26	106.74
3	A	503	86H	C10-C4-C5	-2.66	120.22	123.35
3	A	503	86H	O21-S19-N18	-2.63	100.33	106.74
3	A	503	86H	C16-C15-N18	2.39	125.05	120.02
3	A	503	86H	C14-C15-N18	-2.34	115.09	120.02
3	A	503	86H	C12-C2-N3	2.29	119.34	116.04
3	A	503	86H	C17-C16-C15	-2.23	117.73	120.30

There are no chirality outliers.

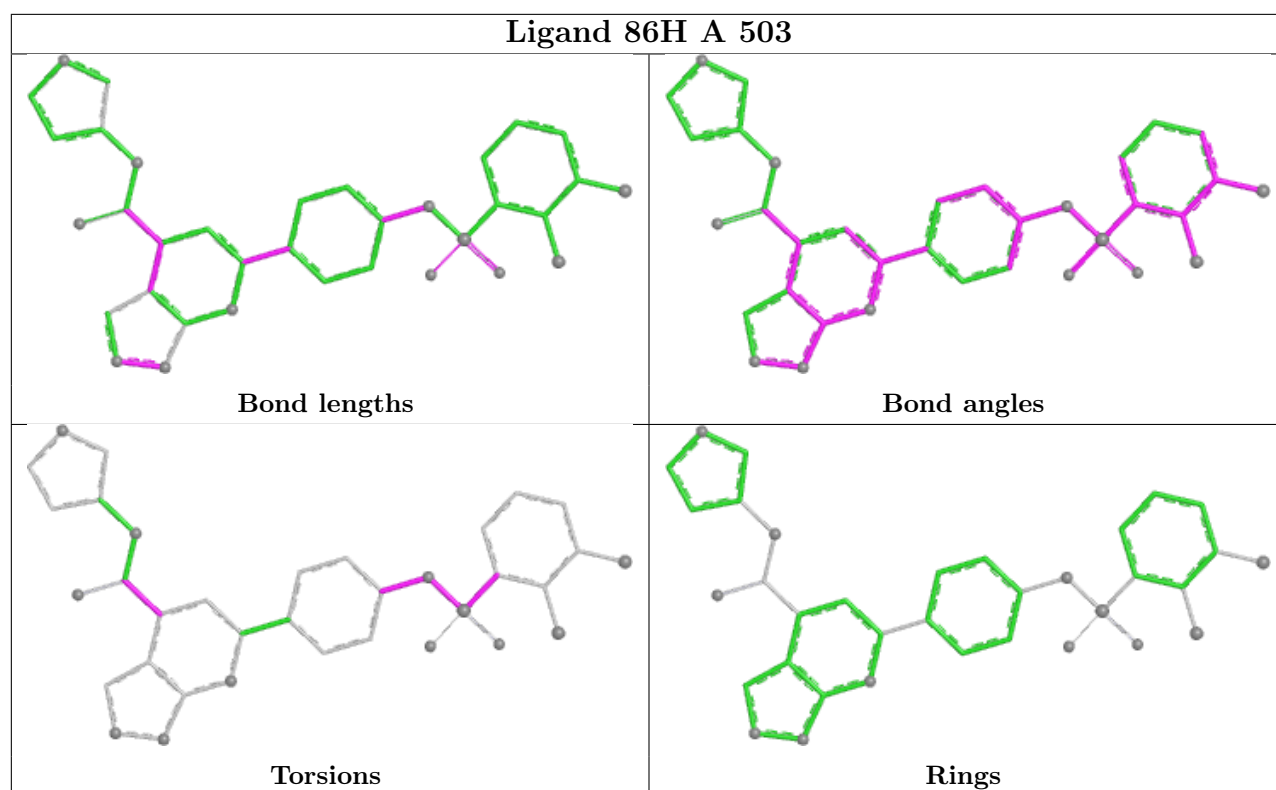
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
3	A	503	86H	N30-C10-C4-C5
3	A	503	86H	O11-C10-C4-C5
3	A	503	86H	N30-C10-C4-C1
3	A	503	86H	O11-C10-C4-C1
3	A	503	86H	C15-N18-S19-C22
3	A	503	86H	C23-C22-S19-N18
3	A	503	86H	C15-N18-S19-O21
2	A	501	GOL	O1-C1-C2-O2
3	A	503	86H	C23-C22-S19-O21
3	A	503	86H	C15-N18-S19-O20
3	A	503	86H	C16-C15-N18-S19
3	A	503	86H	C14-C15-N18-S19

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	271/375 (72%)	0.49	23 (8%) 16 14	50, 79, 142, 162	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	VAL	3.0
1	A	134	ILE	3.0
1	A	120	GLU	2.9
1	A	125	ALA	2.8
1	A	122	VAL	2.6
1	A	243	LEU	2.5
1	A	151	LEU	2.4
1	A	99	HIS	2.3
1	A	192	ALA	2.3
1	A	85	LEU	2.3
1	A	101	LEU	2.3
1	A	121	GLU	2.3
1	A	126	VAL	2.3
1	A	149	VAL	2.3
1	A	245	LYS	2.3
1	A	319	ASN	2.2
1	A	83	ILE	2.2
1	A	180	ASN	2.1
1	A	150	LEU	2.1
1	A	152	LYS	2.1
1	A	169	ALA	2.0
1	A	131	LYS	2.0
1	A	375	ASN	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](#)

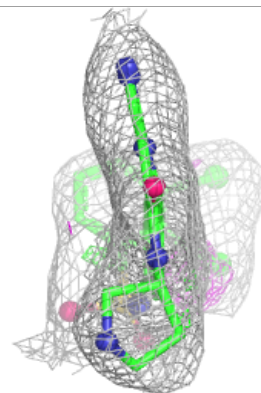
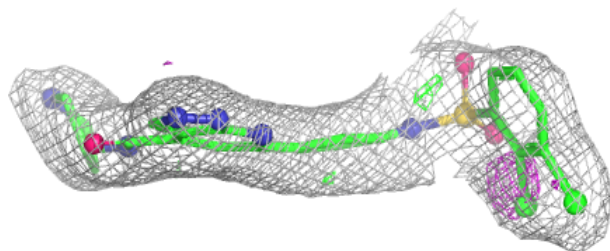
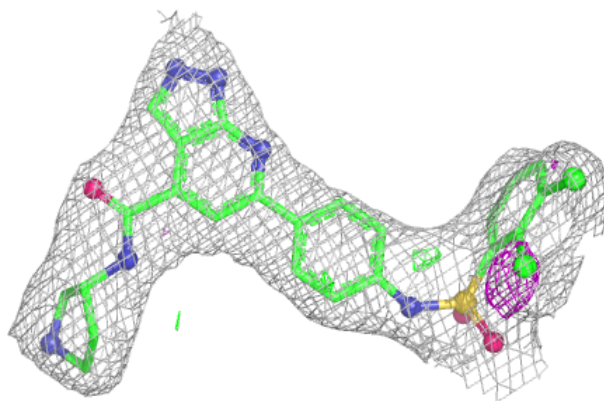
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	502	6/6	0.88	0.11	97,97,97,97	0
2	GOL	A	501	6/6	0.89	0.10	98,99,100,100	0
3	86H	A	503	35/35	0.92	0.10	74,76,85,86	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 86H A 503:

$2mF_o-DF_c$ (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.