



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:11 PM UTC

PDB ID : 4QPS / pdb_00004qps
Title : Crystal structure of Jak3 complexed to N-[3-(6-Phenylamino-pyrazin-2-yl)-3-H-benzoimidazol-5-yl]-acrylamide
Authors : Argiriadi, M.A.; Goedken, E.R.
Deposited on : 2014-06-24
Resolution : 1.80 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

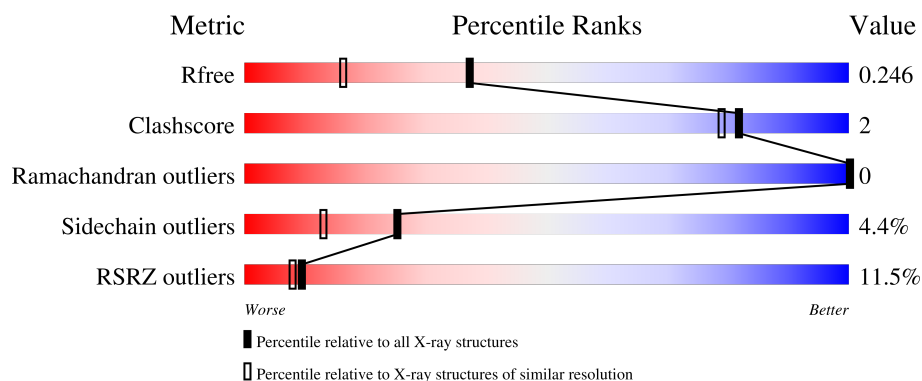
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	293	
1	C	293	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4670 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.

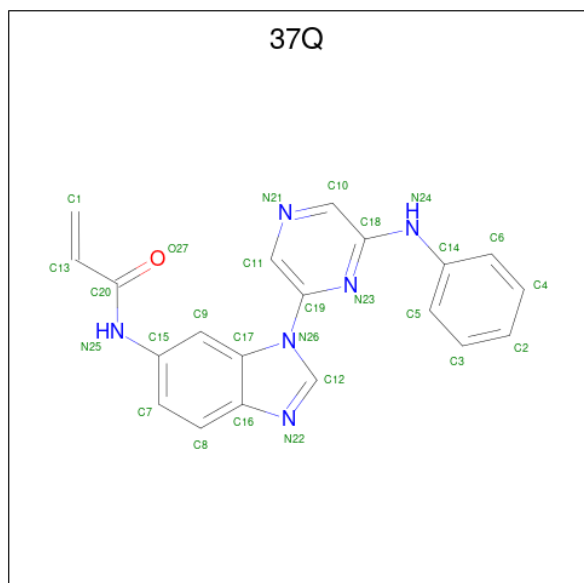
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	4	0
			2189	1401	377	397	14			
1	C	276	Total	C	N	O	S	0	5	0
			2228	1422	385	406	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	949	ALA	ASP	engineered mutation	UNP P52333
A	1040	SER	CYS	engineered mutation	UNP P52333
A	1048	SER	CYS	engineered mutation	UNP P52333
C	949	ALA	ASP	engineered mutation	UNP P52333
C	1040	SER	CYS	engineered mutation	UNP P52333
C	1048	SER	CYS	engineered mutation	UNP P52333

- Molecule 2 is N-{1-[6-(phenylamino)pyrazin-2-yl]-1H-benzimidazol-6-yl}prop-2-enamide (CCD ID: 37Q) (formula: C₂₀H₁₆N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	20	6	1		
2	C	1	Total	C	N	O	0	0
			27	20	6	1		

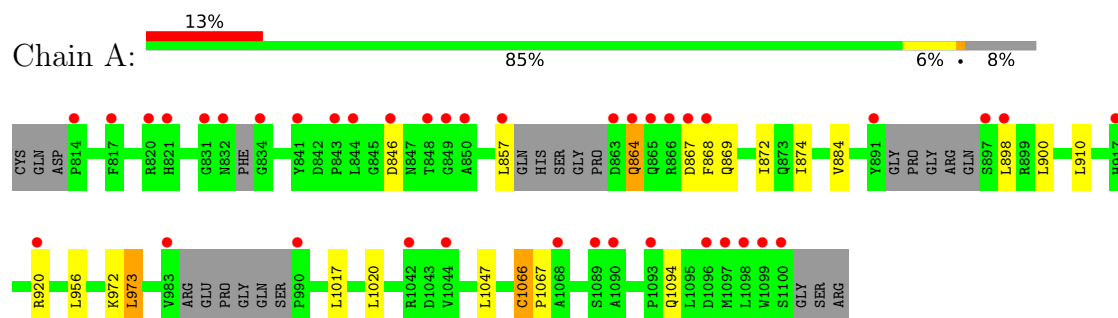
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	C	100	Total	O	0	0
			100	100		

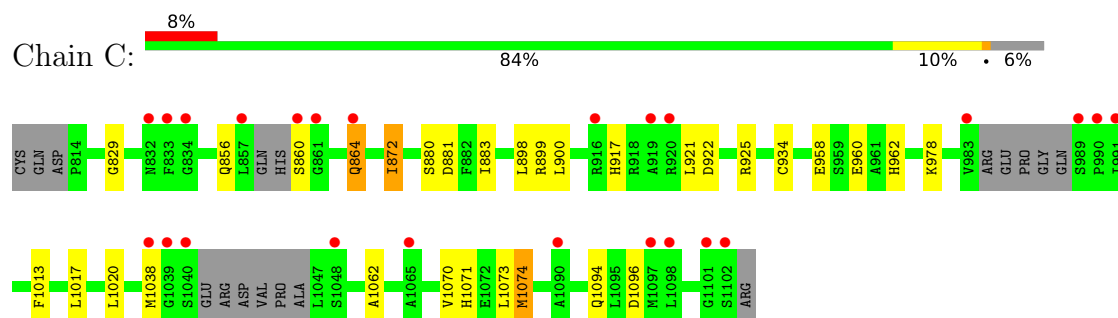
3 Residue-property plots [i](#)

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 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: Tyrosine-protein kinase JAK3



• Molecule 1: Tyrosine-protein kinase JAK3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.51Å 43.88Å 81.69Å 90.00° 115.26° 90.00°	Depositor
Resolution (Å)	39.67 – 1.80 39.67 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.67-1.80) 98.5 (39.67-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 1.81Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.207 , 0.251 0.201 , 0.246	Depositor DCC
R_{free} test set	2382 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4670	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1747e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 37Q

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	0.80	0/2237	1.09	1/3021 (0.0%)
1	C	0.81	1/2279 (0.0%)	1.11	3/3078 (0.1%)
All	All	0.81	1/4516 (0.0%)	1.10	4/6099 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1074	MET	SD-CE	-5.21	1.66	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1066	CYS	N-CA-C	7.17	120.03	109.42
1	C	917	HIS	CA-C-N	5.47	129.03	120.82
1	C	917	HIS	C-N-CA	5.47	129.03	120.82
1	C	922	ASP	CA-CB-CG	5.08	117.68	112.60

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	2189	0	2181	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2228	0	2206	14	0
2	A	27	0	15	1	0
2	C	27	0	14	2	0
3	A	99	0	0	0	0
3	C	100	0	0	0	0
All	All	4670	0	4416	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 2.

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:C:872:ILE:HD13	1:C:900:LEU:HD13	1.50	0.91
1:C:872:ILE:CD1	1:C:900:LEU:HD13	2.21	0.71
1:C:925:ARG:NH1	1:C:960:GLU:HG3	2.07	0.70
1:C:925:ARG:HH12	1:C:960:GLU:HG3	1.56	0.69
1:A:884[B]:VAL:HG21	1:A:956:LEU:HD12	1.78	0.65
1:C:856:GLN:HG3	1:C:899:ARG:HG2	1.77	0.64
1:C:934[B]:CYS:SG	1:C:1013:PHE:CZ	2.93	0.61
1:A:874:ILE:HG12	1:A:973:LEU:HD13	1.87	0.56
1:C:1073:LEU:HD11	1:C:1094:GLN:HG2	1.90	0.53
1:C:881:ASP:O	1:C:962:HIS:HE1	1.91	0.53
1:A:864:GLN:HG3	1:A:867:ASP:HB2	1.91	0.52
1:C:921:LEU:HD22	1:C:925:ARG:HG2	1.91	0.51
2:C:1201:37Q:N23	2:C:1201:37Q:H3	2.26	0.50
1:C:860:SER:N	1:C:864:GLN:HG3	2.27	0.50
1:C:1062:ALA:HB2	1:C:1071:HIS:CG	2.48	0.49
1:A:910:LEU:HD21	1:A:1020:LEU:HD21	1.96	0.47
1:C:829:GLY:HA3	2:C:1201:37Q:H12	1.95	0.47
2:A:1201:37Q:N23	2:A:1201:37Q:H3	2.32	0.45
1:C:1070:VAL:HG12	1:C:1074:MET:HE3	1.99	0.45
1:A:872:ILE:HG13	1:A:900[B]:LEU:HD21	1.99	0.44
1:C:880:SER:HB3	1:C:883[B]:ILE:HD12	1.99	0.43
1:A:1066:CYS:HA	1:A:1067:PRO:HD3	1.98	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	264/293 (90%)	260 (98%)	4 (2%)	0	100	100
1	C	273/293 (93%)	268 (98%)	5 (2%)	0	100	100
All	All	537/586 (92%)	528 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	240/255 (94%)	228 (95%)	12 (5%)	22	10
1	C	244/255 (96%)	235 (96%)	9 (4%)	30	18
All	All	484/510 (95%)	463 (96%)	21 (4%)	25	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	ASP
1	A	857	LEU
1	A	864	GLN
1	A	868	PHE
1	A	869	GLN
1	A	898	LEU
1	A	920	ARG
1	A	972	LYS

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Mol	Chain	Res	Type
1	A	973	LEU
1	A	1017	LEU
1	A	1047	LEU
1	A	1094	GLN
1	C	864	GLN
1	C	872	ILE
1	C	898	LEU
1	C	958	GLU
1	C	978	LYS
1	C	1017	LEU
1	C	1020	LEU
1	C	1038	MET
1	C	1096	ASP

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	864	GLN
1	A	962	HIS
1	A	1071	HIS
1	C	827	GLN
1	C	864	GLN
1	C	865	GLN
1	C	869	GLN
1	C	896	GLN
1	C	962	HIS

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

2 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	37Q	A	1201	1	30,30,30	1.11	1 (3%)	40,41,41	2.99	10 (25%)
2	37Q	C	1201	1	30,30,30	1.16	2 (6%)	40,41,41	2.05	9 (22%)

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	37Q	A	1201	1	-	2/14/14/14	0/4/4/4
2	37Q	C	1201	1	-	3/14/14/14	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	37Q	C1-C13	4.52	1.52	1.30
2	A	1201	37Q	C1-C13	4.20	1.50	1.30
2	C	1201	37Q	C13-C20	2.08	1.51	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	37Q	C1-C13-C20	-14.57	106.21	122.22
2	C	1201	37Q	C1-C13-C20	-8.23	113.18	122.22
2	A	1201	37Q	C13-C20-N25	-7.31	108.88	113.84
2	C	1201	37Q	C18-C10-N21	4.61	124.74	121.75
2	A	1201	37Q	C18-C10-N21	3.32	123.90	121.75
2	A	1201	37Q	O27-C20-N25	3.14	127.25	123.11
2	C	1201	37Q	C10-C18-N23	-2.93	120.34	121.94
2	C	1201	37Q	C11-N21-C10	-2.79	113.72	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	37Q	C11-C19-N26	-2.77	117.98	121.08
2	A	1201	37Q	C15-C9-C17	-2.54	115.16	119.48
2	A	1201	37Q	C7-C8-C16	-2.42	115.94	119.97
2	A	1201	37Q	C7-C15-C9	2.41	122.56	119.66
2	C	1201	37Q	C13-C20-N25	-2.29	112.28	113.84
2	C	1201	37Q	C9-C17-N26	2.24	133.59	130.70
2	C	1201	37Q	N26-C12-N22	-2.21	111.12	114.15
2	A	1201	37Q	C11-N21-C10	-2.20	114.52	117.51
2	A	1201	37Q	C9-C15-N25	-2.18	113.04	120.13
2	C	1201	37Q	C11-C19-N26	-2.14	118.68	121.08
2	C	1201	37Q	C15-N25-C20	-2.11	124.10	128.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

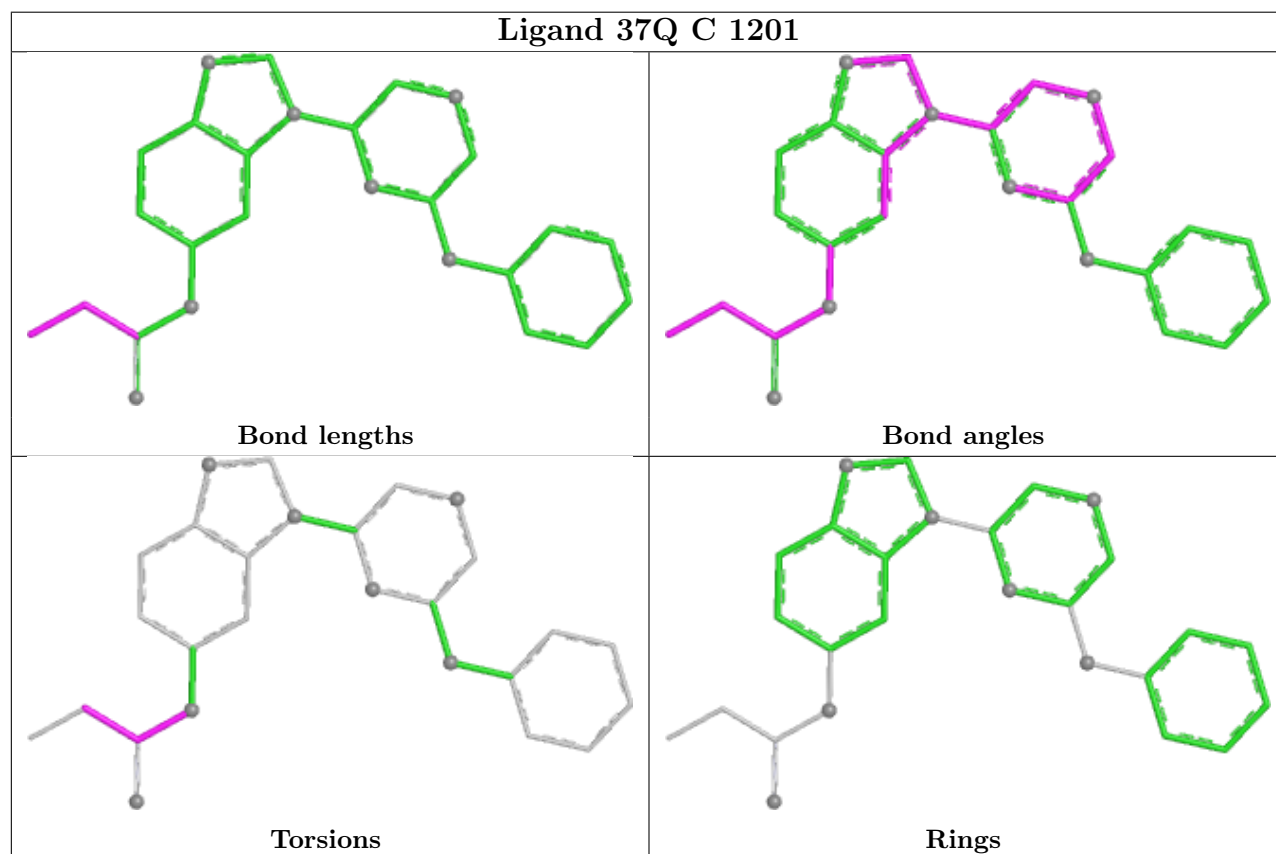
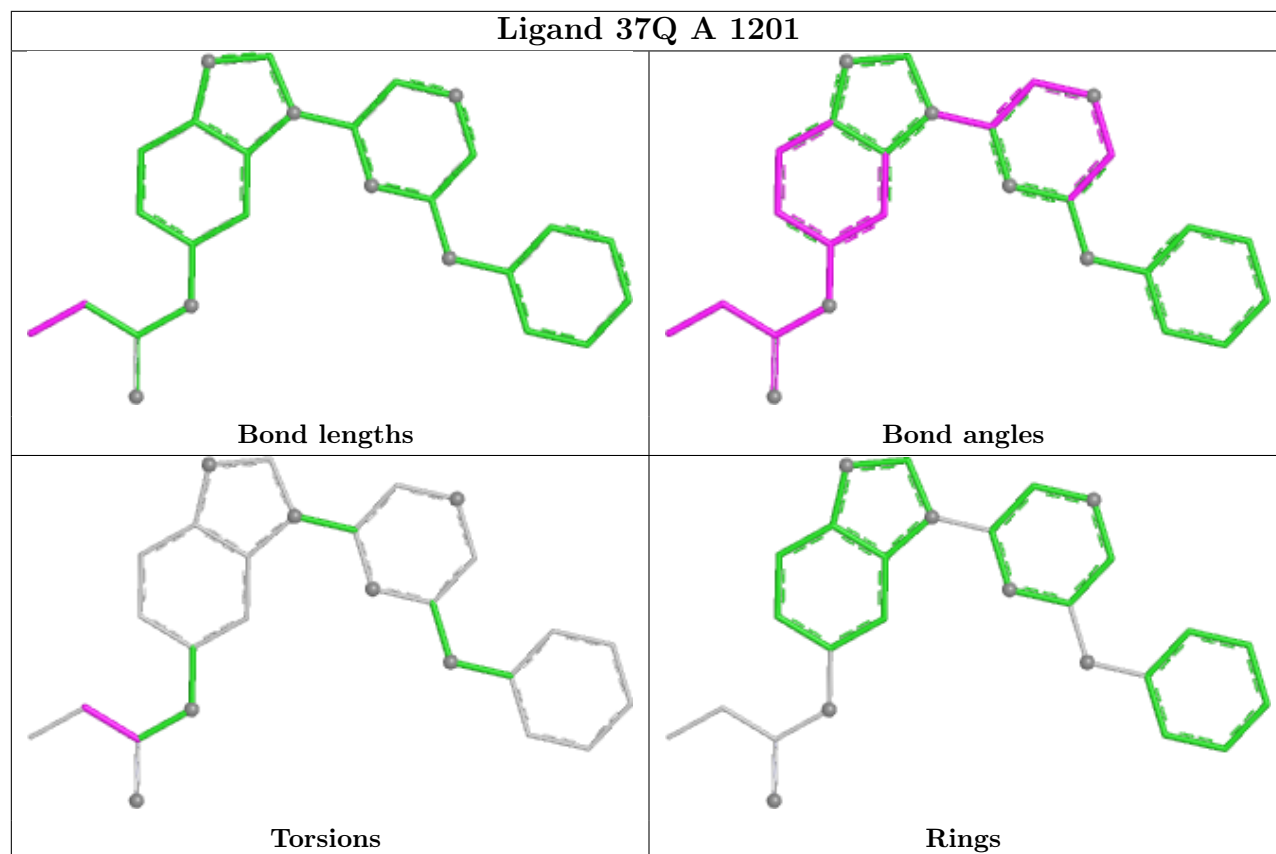
Mol	Chain	Res	Type	Atoms
2	A	1201	37Q	C1-C13-C20-N25
2	A	1201	37Q	C1-C13-C20-O27
2	C	1201	37Q	C1-C13-C20-N25
2	C	1201	37Q	C1-C13-C20-O27
2	C	1201	37Q	O27-C20-N25-C15

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	37Q	1	0
2	C	1201	37Q	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

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	270/293 (92%)	0.64	39 (14%) 6 5	11, 26, 59, 90	6 (2%)
1	C	276/293 (94%)	0.40	24 (8%) 16 14	9, 26, 51, 81	6 (2%)
All	All	546/586 (93%)	0.52	63 (11%) 9 8	9, 26, 54, 90	12 (2%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	844	LEU	9.7
1	A	820	ARG	7.3
1	A	1100	SER	5.9
1	C	1039	GLY	5.5
1	A	1044	VAL	5.1
1	C	1102	SER	5.1
1	A	814	PRO	5.0
1	A	868	PHE	4.7
1	C	833	PHE	4.5
1	C	1040	SER	4.3
1	A	867	ASP	4.2
1	A	866	ARG	4.1
1	A	832	ASN	4.1
1	C	990	PRO	4.1
1	A	1089	SER	4.0
1	A	857	LEU	4.0
1	C	1048	SER	3.9
1	A	891	TYR	3.7
1	A	983	VAL	3.7
1	C	983	VAL	3.7
1	C	1101	GLY	3.6
1	C	989	SER	3.6
1	C	1065	ALA	3.5
1	A	865	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	863	ASP	3.4
1	C	857	LEU	3.0
1	A	1090	ALA	3.0
1	A	834	GLY	3.0
1	A	1097	MET	2.9
1	A	1096	ASP	2.9
1	C	1097	MET	2.9
1	C	1098	LEU	2.8
1	A	1098	LEU	2.8
1	A	1093	PRO	2.8
1	A	1042	ARG	2.7
1	A	897	SER	2.7
1	A	841	TYR	2.7
1	C	834	GLY	2.7
1	C	860	SER	2.6
1	C	920	ARG	2.6
1	A	850	ALA	2.6
1	C	832	ASN	2.6
1	A	848	THR	2.6
1	A	864	GLN	2.4
1	A	1099	TRP	2.4
1	A	920	ARG	2.4
1	A	990	PRO	2.4
1	A	898	LEU	2.4
1	A	849	GLY	2.4
1	A	1068	ALA	2.3
1	C	1038	MET	2.3
1	C	861	GLY	2.3
1	A	917	HIS	2.3
1	C	1090	ALA	2.3
1	A	821	HIS	2.3
1	A	843	PRO	2.2
1	C	991	ILE	2.1
1	A	846	ASP	2.1
1	C	864	GLN	2.1
1	C	919	ALA	2.1
1	C	916	ARG	2.1
1	A	817	PHE	2.0
1	A	831	GLY	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](#)

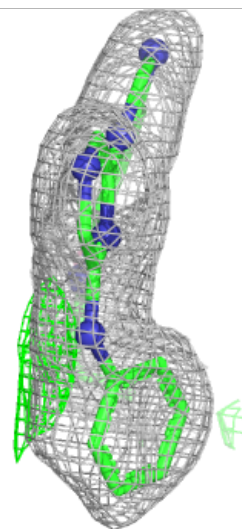
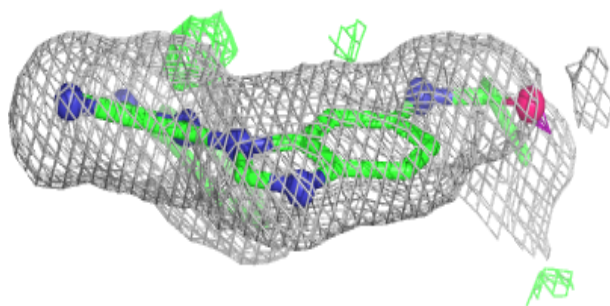
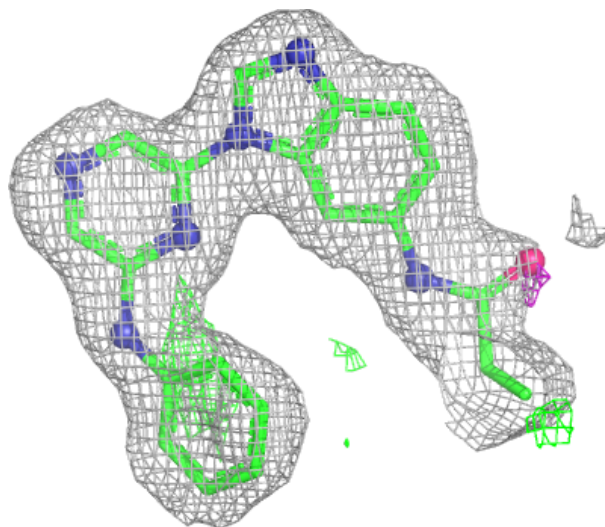
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	37Q	A	1201	27/27	0.93	0.09	19,26,34,43	0
2	37Q	C	1201	27/27	0.97	0.04	16,19,24,28	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.

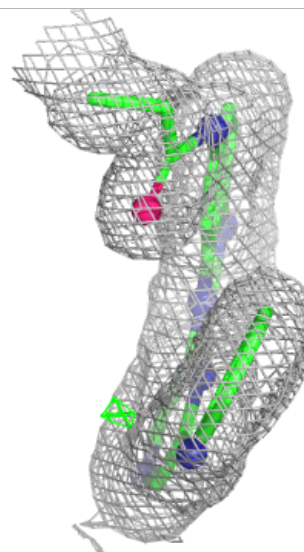
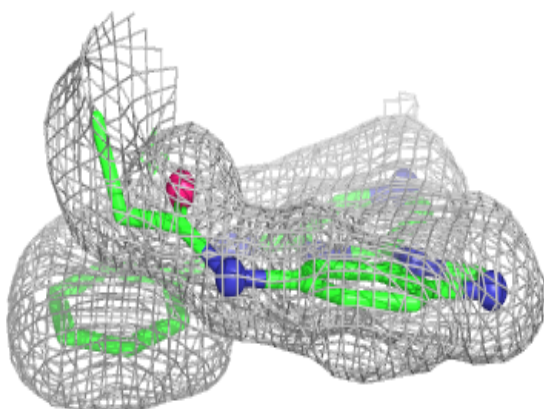
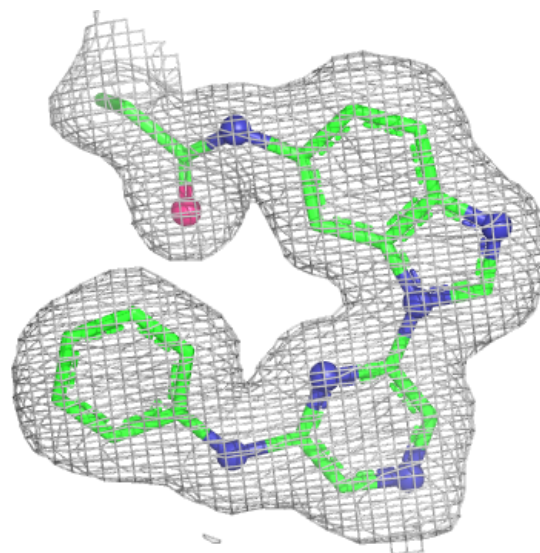
Electron density around 37Q A 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 37Q C 1201:

$2mF_o-DF_c$ (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.