



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 04:07 PM EST

PDB ID : 4OOM
Title : Crystal structure of PBP3 in complex with BAL30072 ((2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-{[(1,5-dihydroxy-4-oxo-1,4-dihydropyridin-2-yl)methoxy]imino}-N-{(2S)-1-hydroxy-3-methyl-3-[(sulfooxy)amino]butan-2-yl}ethanamide)
Authors : Han, S.; Caspers, N.; Knafels, J.D.
Deposited on : 2014-02-03
Resolution : 2.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

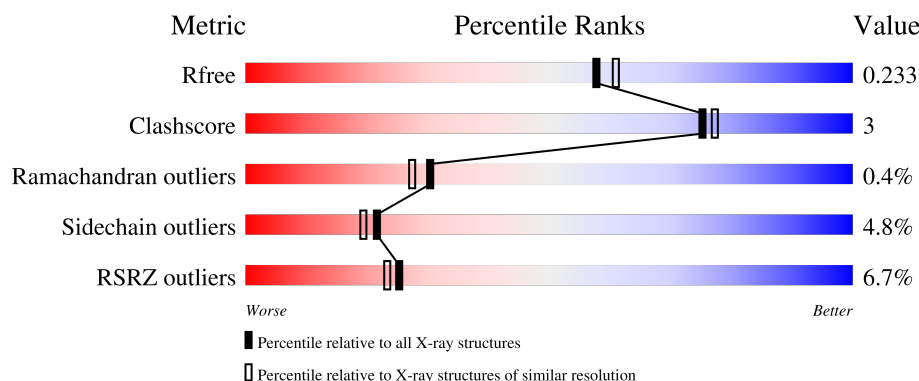
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	538	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4084 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.

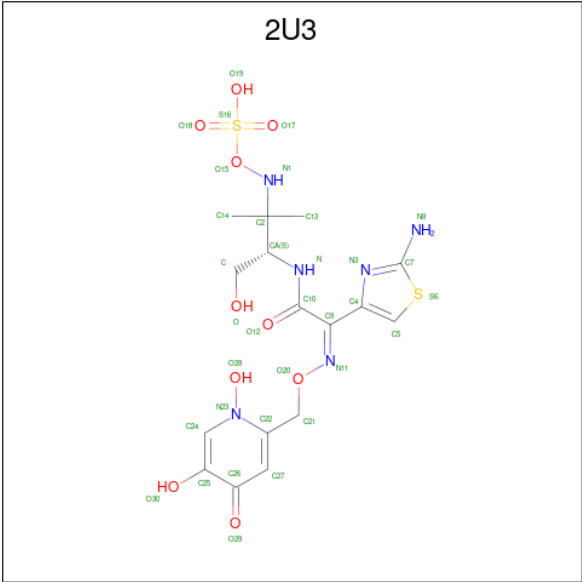
- Molecule 1 is a protein called Cell division protein FtsI [Peptidoglycan synthetase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	1	0
			3791	2393	687	699	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	initiating methionine	UNP U6AVY0
A	43	GLY	-	expression tag	UNP U6AVY0
A	44	HIS	-	expression tag	UNP U6AVY0
A	45	HIS	-	expression tag	UNP U6AVY0
A	46	HIS	-	expression tag	UNP U6AVY0
A	47	HIS	-	expression tag	UNP U6AVY0
A	48	HIS	-	expression tag	UNP U6AVY0
A	49	HIS	-	expression tag	UNP U6AVY0

- Molecule 2 is (2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-[[[(1,5-dihydroxy-4-oxo-1,4-dihydropyridin-2-yl)methoxy]imino}-N-{(2S)-1-hydroxy-3-methyl-3-[(sulfooxy)amino]butan-2-yl}ethanamide (three-letter code: 2U3) (formula: C₁₆H₂₂N₆O₁₀S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	16	6	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	259	Total	O	0	0
			259	259		

- Molecule 1: Cell division protein FtsI [Peptidoglycan synthetase]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.66Å 82.82Å 88.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.52 – 2.00 29.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.52-2.00) 95.8 (29.52-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.00Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.187 , 0.225 0.192 , 0.233	Depositor DCC
R_{free} test set	1655 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4084	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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: 2U3

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	0.48	0/3868	0.66	0/5246

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

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	3791	0	3846	22	0
2	A	34	0	19	0	0
3	A	259	0	0	0	0
All	All	4084	0	3865	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 3.

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:275:ASN:HD22	1:A:276:LEU:N	1.46	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:HD22	1:A:275:ASN:C	1.75	0.87
1:A:275:ASN:C	1:A:275:ASN:ND2	2.28	0.83
1:A:275:ASN:ND2	1:A:276:LEU:N	2.30	0.71
1:A:275:ASN:HD22	1:A:276:LEU:CA	2.04	0.70
1:A:275:ASN:O	1:A:276:LEU:C	2.41	0.58
1:A:264:ASN:HD21	1:A:285:ALA:H	1.54	0.55
1:A:398:PRO:HD2	1:A:401:GLU:HB2	1.87	0.55
1:A:86:PRO:HG3	1:A:123:ILE:HG12	1.91	0.53
1:A:275:ASN:ND2	1:A:276:LEU:CA	2.74	0.51
1:A:239:LEU:HG	1:A:244:ALA:HB3	1.95	0.49
1:A:196:LEU:HD22	1:A:205:LYS:HE3	1.95	0.48
1:A:275:ASN:O	1:A:276:LEU:O	2.32	0.47
1:A:325:ILE:HD12	1:A:399:LYS:HD3	1.97	0.46
1:A:505[B]:SER:OG	1:A:534:GLY:HA2	2.16	0.45
1:A:189:VAL:HG13	1:A:214:LYS:HB2	1.97	0.45
1:A:222:SER:HB2	1:A:258:GLU:HB3	1.99	0.45
1:A:408:GLY:HA2	1:A:411:LEU:HD21	2.00	0.44
1:A:322:THR:HG22	1:A:331:ARG:HG2	2.01	0.43
1:A:117:ASN:HB3	1:A:120:ARG:HD2	2.01	0.43
1:A:169:ASP:HB3	1:A:175:ARG:HG3	1.99	0.43
1:A:175:ARG:HE	1:A:175:ARG:HB3	1.75	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	493/538 (92%)	481 (98%)	10 (2%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	LEU
1	A	207	VAL

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	396/426 (93%)	377 (95%)	19 (5%)	21	19

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ILE
1	A	67	ASP
1	A	153	ARG
1	A	175	ARG
1	A	176	GLU
1	A	189	VAL
1	A	239	LEU
1	A	274	ARG
1	A	275	ASN
1	A	276	LEU
1	A	277	GLN
1	A	315	ILE
1	A	327	ARG
1	A	371	GLN
1	A	411	LEU
1	A	450	SER
1	A	489	ARG
1	A	514	THR
1	A	536	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	264	ASN
1	A	275	ASN
1	A	283	ASN
1	A	420	HIS

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	2U3	A	601	1	27,35,35	1.19	3 (11%)	26,51,51	3.02	11 (42%)

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	2U3	A	601	1	-	9/19/33/33	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2U3	C13-C2	-2.97	1.50	1.53
2	A	601	2U3	C4-C9	-2.45	1.44	1.47
2	A	601	2U3	C14-C2	-2.39	1.51	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	2U3	C27-C22-N23	9.94	122.88	117.11
2	A	601	2U3	C2-CA-N	5.11	117.22	111.84
2	A	601	2U3	C-CA-N	-4.52	102.24	108.83
2	A	601	2U3	C21-C22-C27	-3.75	119.45	123.93
2	A	601	2U3	CA-N-C10	-3.48	117.82	122.98
2	A	601	2U3	O28-N23-C22	3.17	121.01	117.37
2	A	601	2U3	O12-C10-N	3.03	128.44	123.09
2	A	601	2U3	C22-C27-C26	-2.78	117.97	121.86
2	A	601	2U3	O12-C10-C9	-2.73	117.36	120.45
2	A	601	2U3	O19-S16-O18	2.35	116.79	108.56
2	A	601	2U3	O30-C25-C24	2.19	124.54	121.21

There are no chirality outliers.

All (9) torsion outliers are listed below:

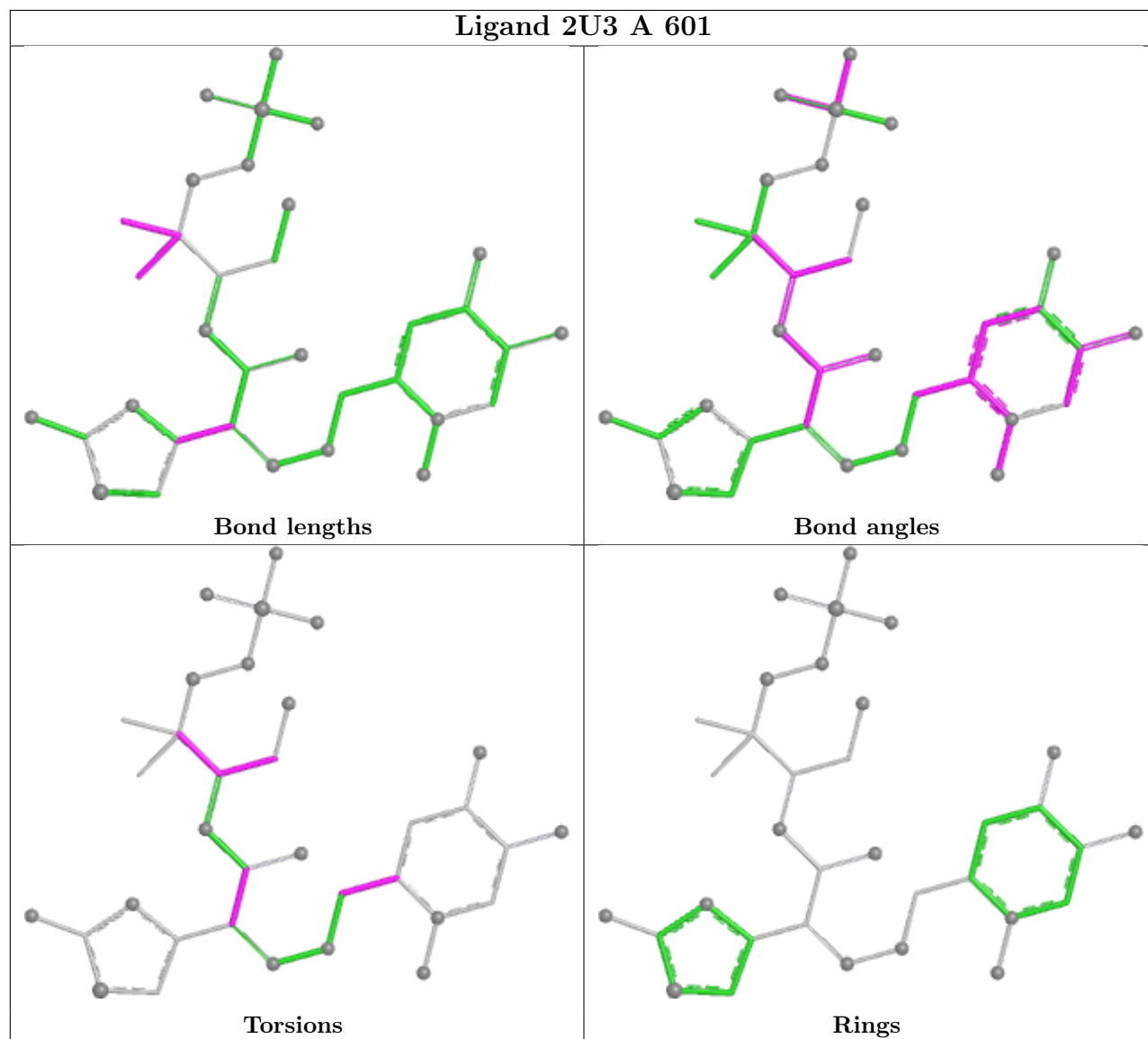
Mol	Chain	Res	Type	Atoms
2	A	601	2U3	O-C-CA-N
2	A	601	2U3	O-C-CA-C2
2	A	601	2U3	C13-C2-CA-N
2	A	601	2U3	C14-C2-CA-N
2	A	601	2U3	C13-C2-CA-C
2	A	601	2U3	C14-C2-CA-C
2	A	601	2U3	O20-C21-C22-C27
2	A	601	2U3	N-C10-C9-N11
2	A	601	2U3	O12-C10-C9-N11

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	496/538 (92%)	0.04	33 (6%) 25 23	18, 32, 90, 152	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	ILE	5.9
1	A	196	LEU	4.7
1	A	203	VAL	4.7
1	A	195	VAL	4.3
1	A	530	ALA	4.3
1	A	205	LYS	3.8
1	A	201	GLY	3.7
1	A	194	GLN	3.6
1	A	207	VAL	3.4
1	A	56	ILE	3.2
1	A	54	ARG	3.2
1	A	197	LYS	3.0
1	A	77	THR	2.8
1	A	532	TYR	2.8
1	A	514	THR	2.8
1	A	276	LEU	2.8
1	A	122	PHE	2.7
1	A	198	ASP	2.7
1	A	229	TYR	2.7
1	A	531	GLY	2.6
1	A	209	VAL	2.5
1	A	124	TYR	2.5
1	A	328	TYR	2.4
1	A	55	HIS	2.4
1	A	273	ARG	2.4
1	A	211	LYS	2.3
1	A	202	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	536	LEU	2.3
1	A	503	TYR	2.2
1	A	192	LYS	2.2
1	A	57	ALA	2.1
1	A	533	PHE	2.1
1	A	200	ARG	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

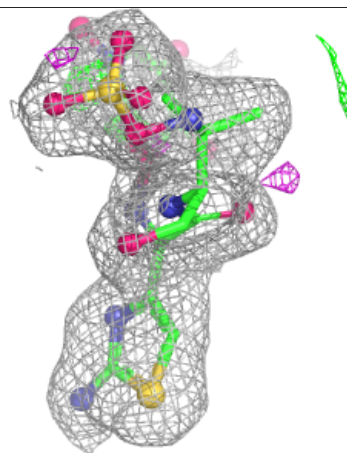
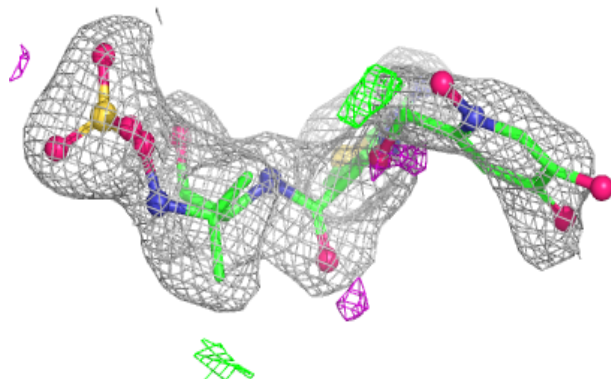
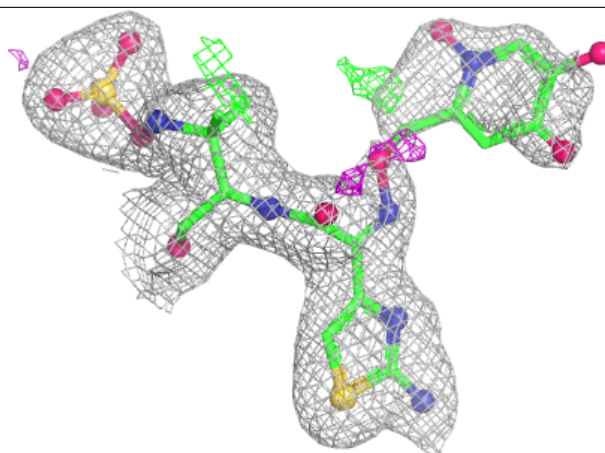
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2U3	A	601	34/34	0.95	0.08	24,36,72,76	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 2U3 A 601:

$2mF_o-DF_c$ (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.