



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:21 pm BST

PDB ID : 4WEK
Title : Crystal structure of Pseudomonas aeruginosa PBP3 with a R4 substituted vinyl monocarbam
Authors : Ferguson, A.D.
Deposited on : 2014-09-10
Resolution : 1.74 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

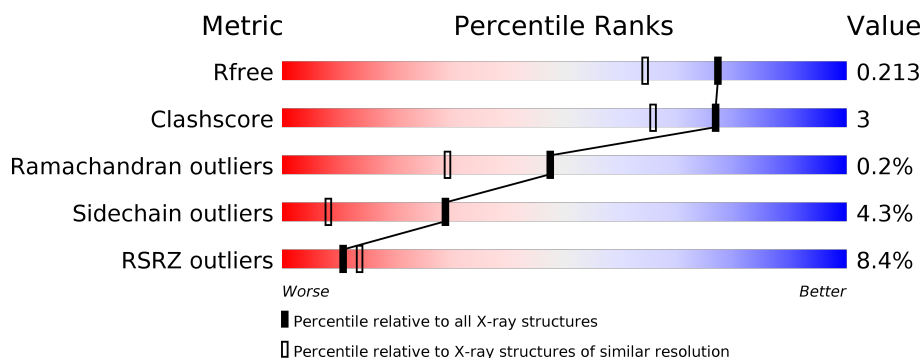
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 on 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	<div> <div>8%</div> <div>84%</div> <div>8% • 7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4191 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.

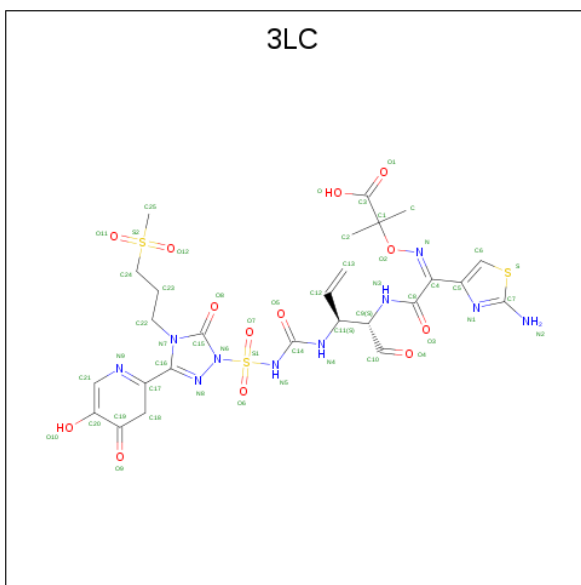
- Molecule 1 is a protein called Penicillin-binding protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	2	0
			3831	2419	695	704	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	MET	-	initiating methionine	UNP K1C6A4
A	287	GLY	-	expression tag	UNP K1C6A4
A	288	HIS	-	expression tag	UNP K1C6A4
A	289	HIS	-	expression tag	UNP K1C6A4
A	290	HIS	-	expression tag	UNP K1C6A4
A	291	HIS	-	expression tag	UNP K1C6A4
A	292	HIS	-	expression tag	UNP K1C6A4
A	293	HIS	-	expression tag	UNP K1C6A4
A	294	SER	ALA	cloning artifact	UNP K1C6A4

- Molecule 2 is (3S,4S,7Z)-7-(2-amino-1,3-thiazol-4-yl)-3-ethenyl-4-formyl-1-[(3-(5-hydroxy-4-oxo-3,4-dihydropyridin-2-yl)-4-[3-(methylsulfonyl)propyl]-5-oxo-4,5-dihydro-1H-1,2,4-triazol-1-yl)sulfonyl]amino]-10,10-dimethyl-1,6-dioxo-9-oxa-2,5,8-triazaundec-7-en-11-oic acid (three-letter code: 3LC) (formula: C₂₆H₃₂N₁₀O₁₃S₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			52	26	10	13	3		

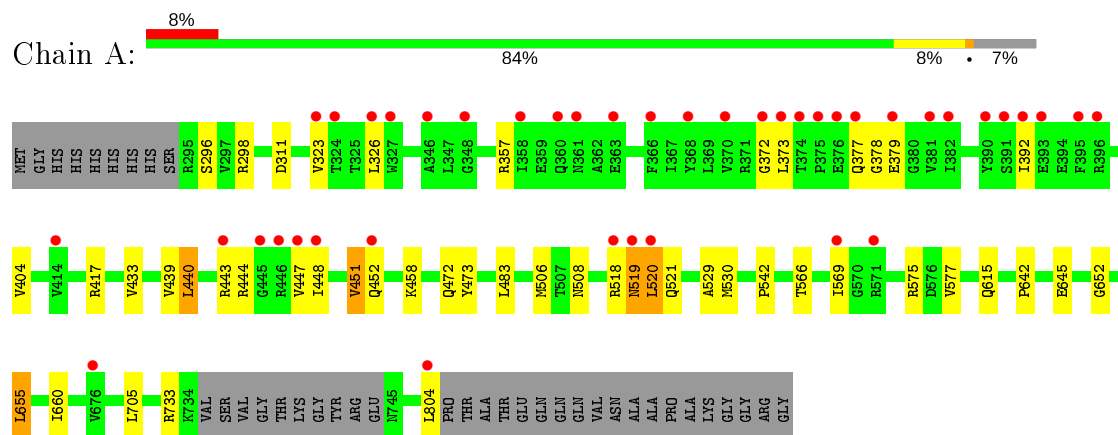
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	308	Total O 308 308	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Penicillin-binding protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.92Å 83.23Å 89.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.71 – 1.74 44.95 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.71-1.74) 99.8 (44.95-1.73)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.73Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.186 , 0.207 0.190 , 0.213	Depositor DCC
R_{free} test set	2755 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.2	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	4191	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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: 3LC

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	0.50	0/3911	0.63	1/5303 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	519	ASN	C-N-CA	6.24	137.30	121.70

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	3831	0	3896	22	0
2	A	52	0	29	2	0
3	A	308	0	0	0	0
All	All	4191	0	3925	23	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 (23) 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:472:GLN:HE22	1:A:506:MET:H	1.29	0.80
1:A:440:LEU:HD13	1:A:448:ILE:HD12	1.78	0.62
1:A:530:MET:HG2	1:A:660:ILE:HG13	1.85	0.59
2:A:901:3LC:H24	2:A:901:3LC:H13	1.86	0.57
1:A:652:GLY:HA2	1:A:655:LEU:HD21	1.89	0.54
1:A:508:ASN:HD21	1:A:529:ALA:H	1.55	0.54
1:A:577:VAL:HG13	2:A:901:3LC:H7	1.91	0.53
1:A:323:VAL:HB	1:A:372:GLY:HA2	1.91	0.52
1:A:439:VAL:HG21	1:A:447:VAL:HG22	1.92	0.52
1:A:439:VAL:CG2	1:A:447:VAL:HG13	2.44	0.47
1:A:451:VAL:HG22	1:A:452:GLN:HG2	1.96	0.46
1:A:373:LEU:HD13	1:A:377:GLN:HB3	1.98	0.46
1:A:519:ASN:CA	1:A:520:LEU:HB2	2.47	0.45
1:A:433:VAL:HG12	1:A:458:LYS:HB3	1.98	0.45
1:A:519:ASN:HA	1:A:520:LEU:CB	2.46	0.44
1:A:404:VAL:HG21	1:A:473:TYR:CE1	2.53	0.44
1:A:326:LEU:HD21	1:A:378:GLY:HA2	1.99	0.43
1:A:642:PRO:HD2	1:A:645:GLU:HB2	1.99	0.43
1:A:542:PRO:HG3	1:A:705:LEU:HD21	2.01	0.43
1:A:566:THR:HG22	1:A:575:ARG:HG2	2.00	0.43
1:A:519:ASN:HA	1:A:520:LEU:HB2	2.03	0.41
1:A:508:ASN:ND2	1:A:529:ALA:H	2.17	0.41
1:A:296:SER:HB3	1:A:298:ARG:CZ	2.51	0.41

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	498/538 (93%)	487 (98%)	10 (2%)	1 (0%)	47 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	LEU

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	401/427 (94%)	384 (96%)	17 (4%)	30 9

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	A	357	ARG
1	A	379	GLU
1	A	392	ILE
1	A	417	ARG
1	A	440	LEU
1	A	443	ARG
1	A	444	ARG
1	A	451	VAL
1	A	483	LEU
1	A	518	ARG
1	A	521	GLN
1	A	569	ILE
1	A	615	GLN
1	A	655	LEU
1	A	733	ARG
1	A	804	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	GLN
1	A	508	ASN
1	A	595	ASN
1	A	671	ASN

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Mol	Chain	Res	Type
1	A	691	GLN
1	A	702	GLN
1	A	706	GLN
1	A	719	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	3LC	A	901	1	37,54,54	1.02	2 (5%)	41,80,80	1.25	3 (7%)

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	3LC	A	901	1	-	6/34/71/71	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	3LC	C13-C12	4.14	1.50	1.29
2	A	901	3LC	C17-N9	2.06	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	901	3LC	C11-C12-C13	-5.64	113.89	124.84
2	A	901	3LC	O9-C19-C18	2.09	124.15	121.12
2	A	901	3LC	C-C1-C3	-2.01	107.16	111.86

There are no chirality outliers.

All (6) torsion outliers are listed below:

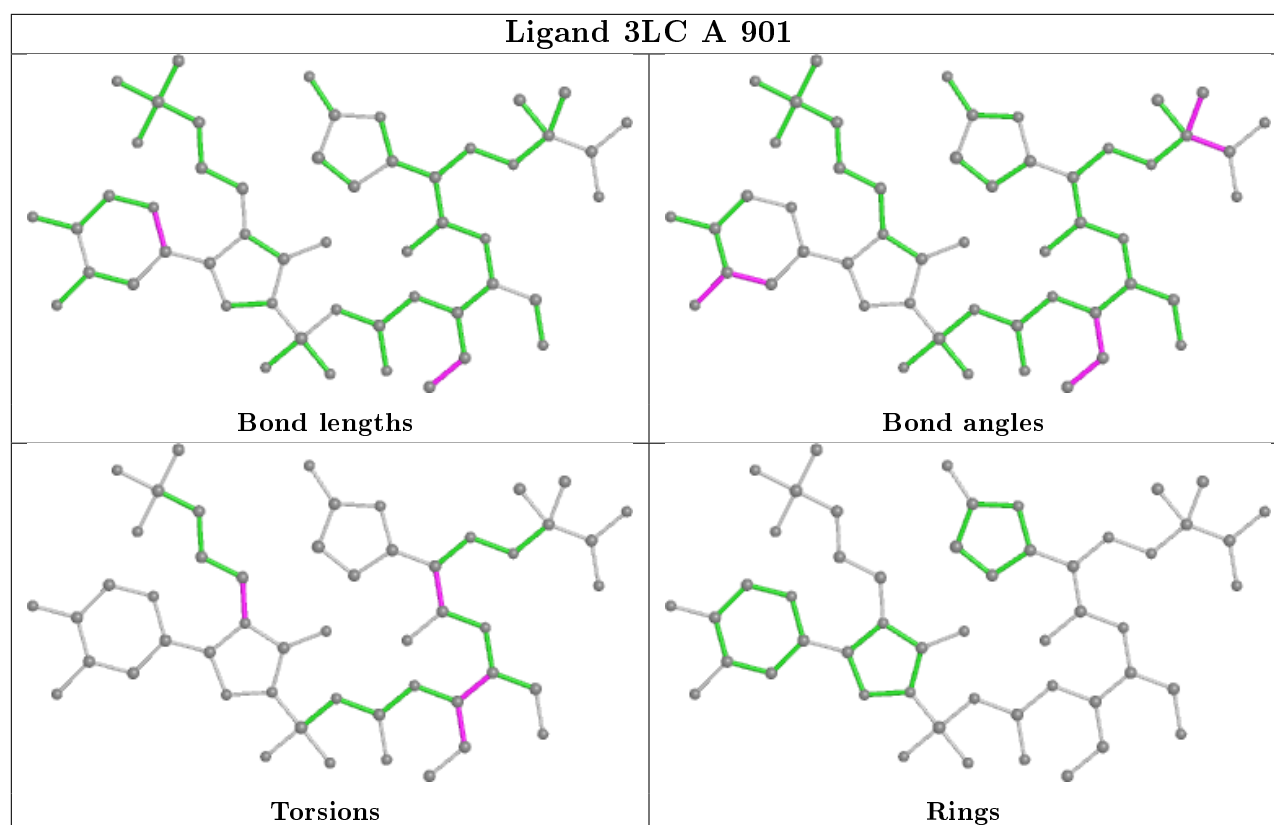
Mol	Chain	Res	Type	Atoms
2	A	901	3LC	C12-C11-C9-N3
2	A	901	3LC	N4-C11-C9-N3
2	A	901	3LC	C9-C11-C12-C13
2	A	901	3LC	N4-C11-C12-C13
2	A	901	3LC	C23-C22-N7-C15
2	A	901	3LC	N-C4-C8-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	3LC	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	500/538 (92%)	0.44	42 (8%) 11 14	18, 30, 61, 89	1 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	GLU	9.1
1	A	376	GLU	7.6
1	A	375	PRO	7.4
1	A	370	VAL	6.9
1	A	372	GLY	6.1
1	A	377	GLN	5.4
1	A	326	LEU	5.2
1	A	374	THR	5.0
1	A	368	TYR	4.6
1	A	346	ALA	4.5
1	A	391	SER	4.3
1	A	520	LEU	4.2
1	A	392	ILE	4.2
1	A	366	PHE	4.1
1	A	395	PHE	4.0
1	A	324	THR	3.7
1	A	348	GLY	3.6
1	A	393	GLU	3.6
1	A	443	ARG	3.5
1	A	519	ASN	3.4
1	A	571	ARG	3.1
1	A	448	ILE	3.0
1	A	518	ARG	2.9
1	A	446	ARG	2.9
1	A	445	GLY	2.8
1	A	414	VAL	2.6
1	A	373	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	390	TYR	2.5
1	A	323	VAL	2.5
1	A	381	VAL	2.5
1	A	361	ASN	2.4
1	A	676	VAL	2.3
1	A	360	GLN	2.2
1	A	396	ARG	2.2
1	A	327	TRP	2.2
1	A	382	ILE	2.1
1	A	452	GLN	2.1
1	A	569	ILE	2.1
1	A	363	GLU	2.0
1	A	447	VAL	2.0
1	A	358	ILE	2.0
1	A	804	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 carbohydrates in this entry.

6.4 Ligands [i](#)

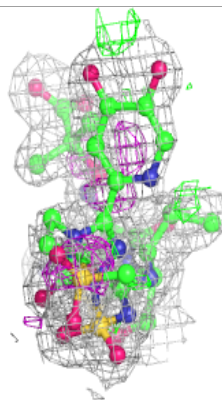
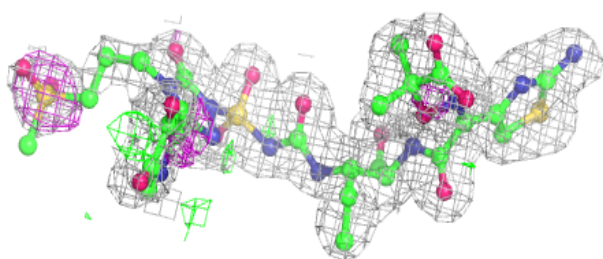
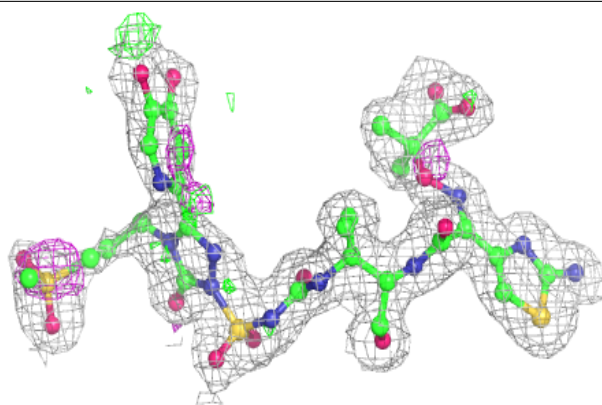
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	3LC	A	901	52/52	0.93	0.12	22,37,56,61	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 3LC A 901:

$2mF_o-DF_c$ (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.