



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2026 – 10:48 am BST

PDB ID : 9RL6 / pdb\_00009rl6  
Title : Structure Guided Optimisation of Niclosamide Derivatives as Direct STAT3 Inhibitors Targeting a Novel Binding Site  
Authors : Quamruzzaman, M.; Maneshi, P.; Knight, R.; Parkinson, G.N.; Wells, G.  
Deposited on : 2025-06-16  
Resolution : 2.55 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](mailto: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>.

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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	:	1.8.4, CSD as541be (2020)
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

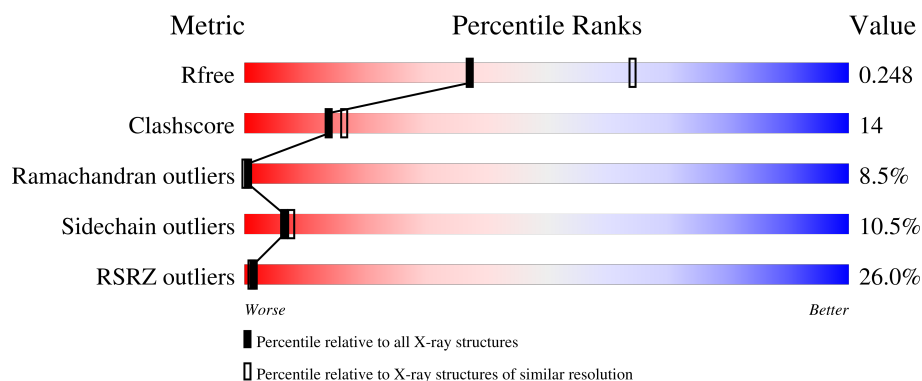
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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  $\geq 3$ , 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	B	18	 78% 22%
2	A	596	 25% 61% 24% 8% 6%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5026 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 DNA chain called DNA (5'-D(\*TP\*GP\*CP\*AP\*TP\*TP\*TP\*CP\*CP\*CP\*GP\*TP\*AP\*AP\*AP\*TP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	18	Total	C	N	O	P	0	0	0
			360	175	59	109	17			

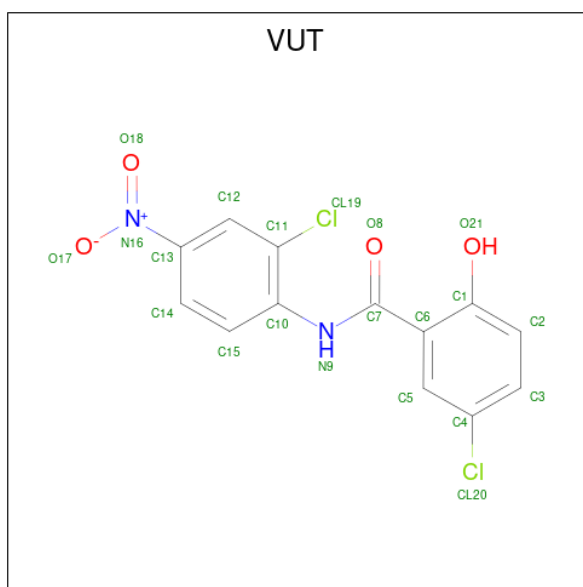
- Molecule 2 is a protein called Isoform Stat3B of Signal transducer and activator of transcription 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	559	Total	C	N	O	S	0	0	0
			4499	2869	766	834	30			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	631	SER	LYS	conflict	UNP P42227

- Molecule 3 is 5-chloro-N-(2-chloro-4-nitrophenyl)-2-hydroxybenzamide (CCD ID: VUT) (formula: C<sub>13</sub>H<sub>8</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			21	13	2	2	4		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	28	Total	O	0	0
			28	28		
4	A	118	Total	O	0	0
			118	118		

### 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.

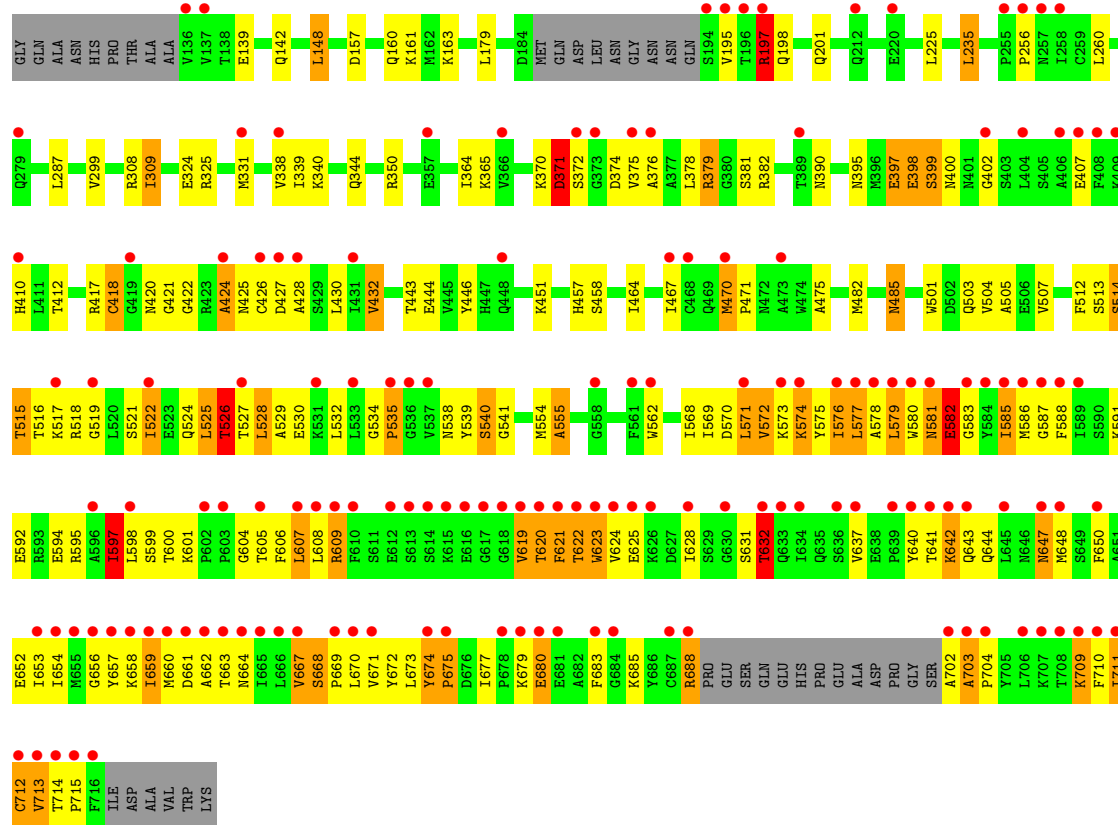
- Molecule 1: DNA (5'-D(\*TP\*GP\*CP\*AP\*TP\*TP\*TP\*CP\*CP\*CP\*GP\*TP\*AP\*AP\*AP\*TP\*CP\*T)-3')

Chain B: 



- Molecule 2: Isoform Stat3B of Signal transducer and activator of transcription 3

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.26Å 174.26Å 78.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.22 – 2.55 123.22 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.5 (123.22-2.55) 96.5 (123.22-2.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, $R_{free}$	0.215 , 0.249 0.219 , 0.248	Depositor DCC
$R_{free}$ test set	1913 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 65.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: VUT

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	B	0.47	0/401	1.17	0/616
2	A	0.57	0/4586	1.07	3/6194 (0.0%)
All	All	0.57	0/4987	1.08	3/6810 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	198	GLN	N-CA-C	-7.32	104.33	113.18
2	A	197	ARG	N-CA-C	-5.80	106.82	114.31
2	A	201	GLN	N-CA-C	-5.20	105.62	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	197	ARG	Sidechain
2	A	308	ARG	Sidechain

## 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	B	360	0	207	2	0
2	A	4499	0	4554	137	2
3	A	21	0	0	2	0
4	A	118	0	0	3	0
4	B	28	0	0	0	0
All	All	5026	0	4761	139	2

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 14.

All (139) 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)
2:A:709:LYS:HE2	2:A:711:ILE:HD11	1.46	0.94
2:A:709:LYS:HE2	2:A:711:ILE:CD1	2.00	0.91
2:A:501:TRP:CZ2	2:A:529:ALA:HB2	2.12	0.84
2:A:518:ARG:HG2	2:A:519:GLY:H	1.49	0.78
2:A:522:ILE:O	2:A:526:THR:HB	1.85	0.77
2:A:672:TYR:HA	2:A:677:ILE:O	1.89	0.73
2:A:597:ILE:CD1	2:A:622:THR:HG21	2.20	0.72
2:A:576:ILE:HG22	2:A:576:ILE:O	1.90	0.71
2:A:524:GLN:HG2	2:A:586:MET:O	1.91	0.71
2:A:641:THR:O	2:A:644:GLN:N	2.23	0.69
2:A:525:LEU:O	2:A:528:LEU:HB3	1.94	0.68
2:A:604:GLY:O	2:A:670:LEU:HB3	1.95	0.66
2:A:573:LYS:O	2:A:574:LYS:C	2.38	0.65
2:A:539:TYR:O	2:A:540:SER:C	2.40	0.65
2:A:382:ARG:CZ	2:A:432:VAL:HG22	2.28	0.64
2:A:669:PRO:HG2	2:A:679:LYS:HE3	1.81	0.63
2:A:325:ARG:NH2	2:A:407:GLU:OE2	2.31	0.63
2:A:648:MET:HE1	2:A:711:ILE:HG23	1.80	0.63
2:A:518:ARG:HG2	2:A:519:GLY:N	2.14	0.62
2:A:679:LYS:HG3	2:A:679:LYS:O	1.99	0.62
2:A:371:ASP:OD1	2:A:371:ASP:C	2.42	0.61
2:A:576:ILE:HD11	2:A:619:VAL:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:378:LEU:HD11	4:A:976:HOH:O	2.00	0.60
2:A:530:GLU:O	2:A:534:GLY:N	2.33	0.60
2:A:417:ARG:O	2:A:418:CYS:HB2	2.01	0.60
2:A:501:TRP:CE2	2:A:529:ALA:HB2	2.36	0.60
2:A:370:LYS:O	2:A:372:SER:N	2.28	0.59
2:A:709:LYS:HE2	2:A:711:ILE:HD13	1.83	0.59
2:A:597:ILE:HD13	2:A:622:THR:HG21	1.85	0.59
2:A:395:ASN:OD1	2:A:397:GLU:HB2	2.02	0.59
2:A:606:PHE:O	2:A:674:TYR:N	2.35	0.59
2:A:658:LYS:O	2:A:659:ILE:HD12	2.03	0.59
2:A:609:ARG:O	2:A:620:THR:N	2.35	0.58
2:A:157:ASP:O	2:A:161:LYS:HG3	2.04	0.57
2:A:605:THR:HA	2:A:672:TYR:O	2.04	0.57
2:A:674:TYR:O	2:A:675:PRO:C	2.47	0.57
2:A:382:ARG:CZ	2:A:432:VAL:CG2	2.83	0.56
2:A:713:VAL:HG12	2:A:713:VAL:O	2.05	0.56
2:A:580:TRP:HA	2:A:585:ILE:HG13	1.88	0.55
2:A:641:THR:O	2:A:642:LYS:C	2.50	0.55
2:A:641:THR:O	2:A:643:GLN:N	2.40	0.55
2:A:623:TRP:CZ3	2:A:659:ILE:HD13	2.41	0.55
2:A:568:ILE:O	2:A:571:LEU:HB3	2.08	0.54
2:A:598:LEU:HD13	2:A:624:VAL:HG13	1.88	0.54
2:A:571:LEU:C	2:A:571:LEU:HD13	2.33	0.53
2:A:378:LEU:HD12	2:A:381:SER:OG	2.08	0.53
2:A:457:HIS:HD2	2:A:458:SER:O	1.90	0.53
2:A:658:LYS:O	2:A:668:SER:N	2.41	0.53
2:A:703:ALA:N	2:A:704:PRO:CD	2.72	0.52
2:A:576:ILE:O	2:A:576:ILE:CG2	2.58	0.52
2:A:525:LEU:O	2:A:526:THR:C	2.52	0.52
2:A:139:GLU:O	2:A:142:GLN:HB2	2.09	0.52
2:A:607:LEU:O	2:A:621:PHE:HA	2.09	0.52
2:A:517:LYS:HD2	2:A:581:ASN:CG	2.35	0.52
2:A:688:ARG:C	4:A:966:HOH:O	2.52	0.52
2:A:505:ALA:HB1	2:A:525:LEU:HD21	1.91	0.51
2:A:591:LYS:HA	2:A:594:GLU:HB3	1.92	0.51
2:A:325:ARG:HG2	2:A:325:ARG:HH11	1.74	0.51
2:A:378:LEU:H	2:A:378:LEU:HD23	1.74	0.51
2:A:324:GLU:O	3:A:801:VUT:C3	2.59	0.51
2:A:650:PHE:HA	2:A:653:ILE:HD12	1.93	0.51
2:A:597:ILE:HD12	2:A:622:THR:HG21	1.92	0.50
2:A:430:LEU:HA	4:A:920:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:482:MET:SD	2:A:507:VAL:HG21	2.52	0.50
2:A:365:LYS:HE2	2:A:390:ASN:HD22	1.77	0.50
2:A:539:TYR:O	2:A:541:GLY:N	2.44	0.50
2:A:672:TYR:HA	2:A:677:ILE:C	2.38	0.49
2:A:324:GLU:OE1	2:A:350:ARG:HD3	2.12	0.49
2:A:572:VAL:O	2:A:572:VAL:HG13	2.11	0.49
2:A:647:ASN:N	2:A:647:ASN:OD1	2.46	0.49
2:A:679:LYS:O	2:A:680:GLU:CB	2.60	0.49
2:A:576:ILE:CD1	2:A:619:VAL:HG21	2.42	0.49
2:A:579:LEU:HD12	2:A:579:LEU:H	1.77	0.48
1:B:3:DC:H2''	1:B:4:DA:OP2	2.13	0.48
2:A:595:ARG:O	2:A:599:SER:HB3	2.14	0.48
2:A:578:ALA:O	2:A:581:ASN:CB	2.62	0.48
2:A:525:LEU:O	2:A:527:THR:N	2.47	0.48
2:A:582:GLU:HB2	2:A:583:GLY:H	1.45	0.47
2:A:667:VAL:HG12	2:A:668:SER:HB3	1.96	0.47
2:A:554:MET:O	2:A:555:ALA:C	2.56	0.47
2:A:640:TYR:HB3	2:A:644:GLN:HB2	1.96	0.47
2:A:702:ALA:O	2:A:703:ALA:HB3	2.15	0.47
2:A:427:ASP:O	2:A:428:ALA:HB3	2.14	0.47
2:A:379:ARG:HH11	2:A:379:ARG:HA	1.81	0.46
2:A:657:TYR:HD1	2:A:713:VAL:HG22	1.81	0.46
2:A:703:ALA:N	2:A:704:PRO:HD3	2.31	0.46
2:A:587:GLY:HA2	2:A:609:ARG:HA	1.98	0.46
2:A:344:GLN:OE1	2:A:410:HIS:ND1	2.49	0.45
2:A:148:LEU:HD12	2:A:148:LEU:HA	1.88	0.45
2:A:679:LYS:O	2:A:679:LYS:CG	2.65	0.45
2:A:522:ILE:HA	2:A:525:LEU:HB3	1.98	0.44
2:A:597:ILE:O	2:A:601:LYS:N	2.32	0.44
2:A:475:ALA:HB2	2:A:562:TRP:CD1	2.51	0.44
1:B:17:DC:H1'	1:B:18:DT:H5'	1.98	0.44
2:A:605:THR:HG22	2:A:672:TYR:HB2	2.00	0.44
2:A:673:LEU:O	2:A:674:TYR:C	2.60	0.44
2:A:324:GLU:O	3:A:801:VUT:C2	2.66	0.44
2:A:604:GLY:HA2	2:A:670:LEU:HD12	2.00	0.44
2:A:424:ALA:O	2:A:425:ASN:HB2	2.18	0.44
2:A:648:MET:HG3	2:A:652:GLU:HG2	2.00	0.44
2:A:517:LYS:HD2	2:A:581:ASN:CB	2.48	0.43
2:A:631:SER:O	2:A:632:THR:OG1	2.27	0.43
2:A:661:ASP:O	2:A:663:THR:N	2.44	0.43
2:A:578:ALA:O	2:A:581:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:514:SER:O	2:A:516:THR:N	2.51	0.43
2:A:517:LYS:NZ	2:A:577:LEU:O	2.51	0.43
2:A:365:LYS:HE2	2:A:390:ASN:ND2	2.34	0.43
2:A:527:THR:OG1	2:A:588:PHE:O	2.34	0.43
2:A:371:ASP:OD1	2:A:372:SER:N	2.52	0.43
2:A:340:LYS:HA	2:A:464:ILE:O	2.18	0.43
2:A:521:SER:N	2:A:524:GLN:OE1	2.43	0.43
2:A:518:ARG:CG	2:A:519:GLY:N	2.81	0.42
2:A:517:LYS:HD2	2:A:581:ASN:HB2	2.01	0.42
2:A:378:LEU:HD23	2:A:378:LEU:N	2.34	0.42
2:A:397:GLU:C	2:A:399:SER:H	2.27	0.42
2:A:650:PHE:CE2	2:A:654:ILE:HD11	2.54	0.42
2:A:400:ASN:C	2:A:402:GLY:H	2.28	0.42
2:A:674:TYR:HB3	2:A:675:PRO:HD3	2.01	0.42
2:A:338:VAL:C	2:A:339:ILE:HD13	2.44	0.41
2:A:235:LEU:HA	2:A:235:LEU:HD23	1.80	0.41
2:A:688:ARG:N	2:A:688:ARG:HD2	2.34	0.41
2:A:364:ILE:HD13	2:A:443:THR:HB	2.02	0.41
2:A:485:ASN:C	2:A:485:ASN:HD22	2.28	0.41
2:A:397:GLU:O	2:A:399:SER:N	2.52	0.41
2:A:446:TYR:CE2	2:A:451:LYS:HG3	2.56	0.41
2:A:467:ILE:HA	2:A:467:ILE:HD12	1.86	0.41
2:A:512:PHE:HB3	2:A:519:GLY:HA2	2.03	0.41
2:A:470:MET:N	2:A:471:PRO:CD	2.84	0.41
2:A:578:ALA:O	2:A:581:ASN:HB2	2.21	0.40
2:A:623:TRP:CZ3	2:A:659:ILE:CD1	3.03	0.40
2:A:309:ILE:HD12	2:A:309:ILE:HA	1.81	0.40
2:A:482:MET:HE1	2:A:504:VAL:HG22	2.03	0.40
2:A:532:LEU:HD23	2:A:532:LEU:HA	1.88	0.40
2:A:621:PHE:CE1	2:A:637:VAL:HG12	2.56	0.40
2:A:580:TRP:CD1	2:A:581:ASN:N	2.89	0.40
2:A:641:THR:O	2:A:644:GLN:HG2	2.20	0.40
2:A:608:LEU:HD11	2:A:683:PHE:CZ	2.56	0.40
2:A:512:PHE:CB	2:A:519:GLY:HA2	2.51	0.40
2:A:710:PHE:C	2:A:711:ILE:HG12	2.47	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:711:ILE:O	2:A:711:ILE:O[6_665]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:709:LYS:O	2:A:712:CYS:SG[6_665]	2.13	0.07

## 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
2	A	553/596 (93%)	458 (83%)	48 (9%)	47 (8%)	<b>0</b> <b>0</b>

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	256	PRO
2	A	398	GLU
2	A	418	CYS
2	A	525	LEU
2	A	526	THR
2	A	540	SER
2	A	570	ASP
2	A	571	LEU
2	A	574	LYS
2	A	579	LEU
2	A	582	GLU
2	A	600	THR
2	A	625	GLU
2	A	659	ILE
2	A	674	TYR
2	A	703	ALA
2	A	714	THR
2	A	371	ASP
2	A	375	VAL
2	A	426	CYS
2	A	514	SER
2	A	528	LEU

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Mol	Chain	Res	Type
2	A	538	ASN
2	A	577	LEU
2	A	581	ASN
2	A	667	VAL
2	A	680	GLU
2	A	515	THR
2	A	535	PRO
2	A	597	ILE
2	A	664	ASN
2	A	715	PRO
2	A	555	ALA
2	A	632	THR
2	A	642	LYS
2	A	374	ASP
2	A	376	ALA
2	A	422	GLY
2	A	424	ALA
2	A	623	TRP
2	A	662	ALA
2	A	421	GLY
2	A	675	PRO
2	A	576	ILE
2	A	569	ILE
2	A	713	VAL
2	A	656	GLY

### 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
2	A	504/534 (94%)	451 (90%)	53 (10%)	<b>6</b> <b>8</b>

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	148	LEU

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Mol	Chain	Res	Type
2	A	160	GLN
2	A	163	LYS
2	A	179	LEU
2	A	195	VAL
2	A	197	ARG
2	A	225	LEU
2	A	235	LEU
2	A	260	LEU
2	A	287	LEU
2	A	299	VAL
2	A	309	ILE
2	A	331	MET
2	A	371	ASP
2	A	379	ARG
2	A	397	GLU
2	A	398	GLU
2	A	399	SER
2	A	412	THR
2	A	420	ASN
2	A	432	VAL
2	A	444	GLU
2	A	470	MET
2	A	485	ASN
2	A	503	GLN
2	A	513	SER
2	A	515	THR
2	A	522	ILE
2	A	526	THR
2	A	535	PRO
2	A	572	VAL
2	A	575	TYR
2	A	582	GLU
2	A	585	ILE
2	A	592	GLU
2	A	597	ILE
2	A	607	LEU
2	A	609	ARG
2	A	619	VAL
2	A	620	THR
2	A	621	PHE
2	A	622	THR
2	A	628	ILE

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Mol	Chain	Res	Type
2	A	632	THR
2	A	647	ASN
2	A	660	MET
2	A	668	SER
2	A	671	VAL
2	A	685	LYS
2	A	688	ARG
2	A	709	LYS
2	A	711	ILE
2	A	712	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	149	GLN
2	A	160	GLN
2	A	167	ASN
2	A	257	ASN
2	A	279	GLN
2	A	288	GLN
2	A	385	ASN
2	A	416	GLN
2	A	448	GLN
2	A	457	HIS
2	A	485	ASN
2	A	538	ASN
2	A	553	ASN
2	A	635	GLN

### 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

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
3	VUT	A	801	-	21,22,22	0.75	0	29,31,31	0.93	1 (3%)

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
3	VUT	A	801	-	-	4/10/12/12	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	VUT	C2-C1-C6	2.12	122.17	119.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

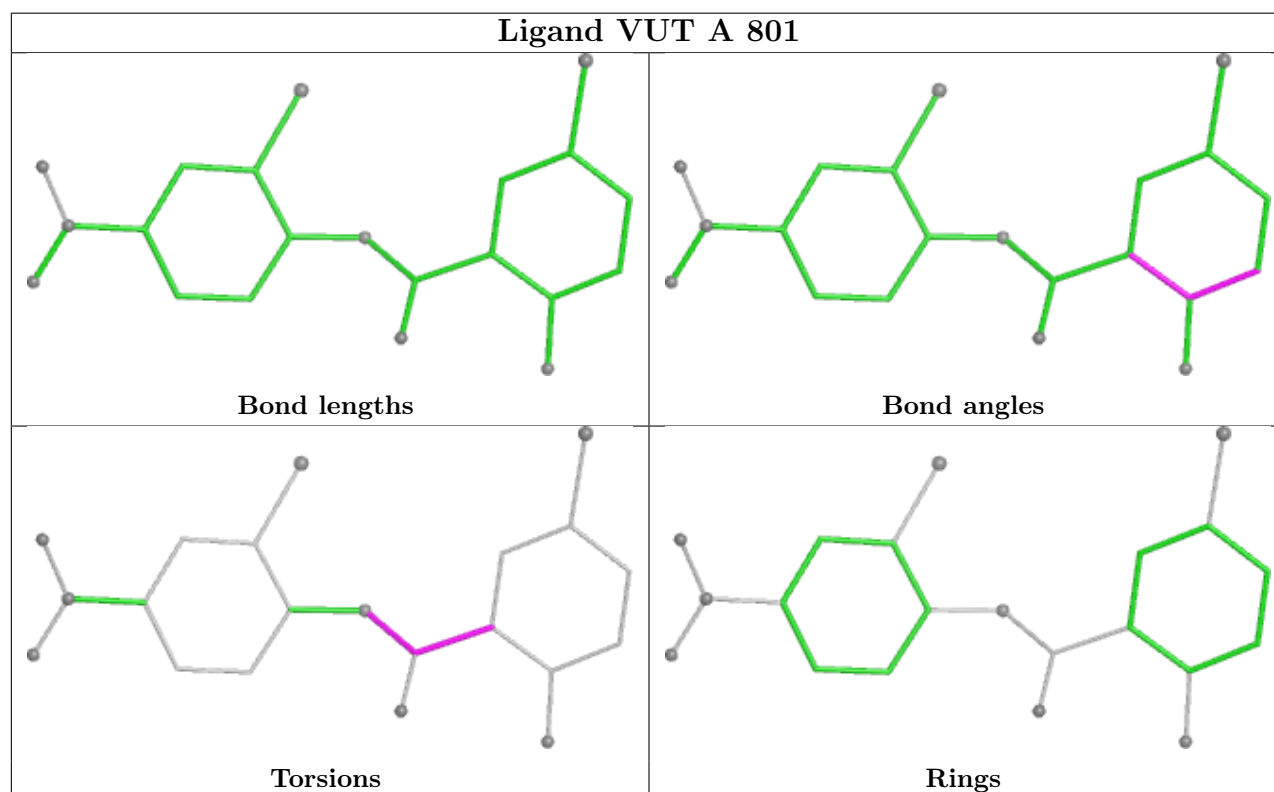
Mol	Chain	Res	Type	Atoms
3	A	801	VUT	C1-C6-C7-O8
3	A	801	VUT	C1-C6-C7-N9
3	A	801	VUT	C6-C7-N9-C10
3	A	801	VUT	O8-C7-N9-C10

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	VUT	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	18/18 (100%)	-0.31	0 100 100	52, 64, 85, 100	0
2	A	559/596 (93%)	1.29	150 (26%) 1 1	47, 82, 167, 217	0
All	All	577/614 (93%)	1.24	150 (25%) 1 1	47, 81, 166, 217	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	656	GLY	9.7
2	A	640	TYR	7.9
2	A	716	PHE	7.5
2	A	710	PHE	7.3
2	A	624	VAL	7.3
2	A	579	LEU	7.2
2	A	637	VAL	6.8
2	A	665	ILE	6.6
2	A	713	VAL	6.6
2	A	195	VAL	6.3
2	A	711	ILE	6.2
2	A	426	CYS	6.1
2	A	619	VAL	6.0
2	A	715	PRO	5.8
2	A	578	ALA	5.8
2	A	666	LEU	5.6
2	A	706	LEU	5.5
2	A	427	ASP	5.5
2	A	655	MET	5.3
2	A	136	VAL	5.2
2	A	375	VAL	5.2
2	A	660	MET	5.2
2	A	630	GLY	5.0
2	A	584	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
2	A	626	LYS	5.0
2	A	194	SER	4.9
2	A	622	THR	4.9
2	A	618	GLY	4.8
2	A	598	LEU	4.7
2	A	257	ASN	4.4
2	A	196	THR	4.4
2	A	642	LYS	4.4
2	A	662	ALA	4.4
2	A	596	ALA	4.3
2	A	664	ASN	4.3
2	A	650	PHE	4.1
2	A	617	GLY	4.1
2	A	197	ARG	4.1
2	A	667	VAL	4.0
2	A	702	ALA	3.9
2	A	671	VAL	3.9
2	A	621	PHE	3.9
2	A	537	VAL	3.9
2	A	688	ARG	3.8
2	A	663	THR	3.8
2	A	585	ILE	3.7
2	A	628	ILE	3.7
2	A	623	TRP	3.7
2	A	402	GLY	3.6
2	A	620	THR	3.6
2	A	220	GLU	3.6
2	A	709	LYS	3.5
2	A	588	PHE	3.5
2	A	703	ALA	3.5
2	A	714	THR	3.4
2	A	607	LEU	3.4
2	A	428	ALA	3.4
2	A	647	ASN	3.4
2	A	608	LEU	3.3
2	A	373	GLY	3.3
2	A	522	ILE	3.3
2	A	639	PRO	3.3
2	A	648	MET	3.3
2	A	707	LYS	3.3
2	A	657	TYR	3.3
2	A	632	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	212	GLN	3.2
2	A	712	CYS	3.2
2	A	679	LYS	3.2
2	A	678	PRO	3.2
2	A	589	ILE	3.2
2	A	574	LYS	3.1
2	A	389	THR	3.1
2	A	609	ARG	3.1
2	A	517	LYS	3.1
2	A	605	THR	3.0
2	A	424	ALA	3.0
2	A	687	CYS	3.0
2	A	683	PHE	3.0
2	A	580	TRP	3.0
2	A	577	LEU	3.0
2	A	614	SER	2.9
2	A	338	VAL	2.9
2	A	670	LEU	2.9
2	A	661	ASP	2.9
2	A	558	GLY	2.9
2	A	527	THR	2.9
2	A	571	LEU	2.8
2	A	366	VAL	2.8
2	A	643	GLN	2.8
2	A	409	LYS	2.8
2	A	616	GLU	2.8
2	A	680	GLU	2.8
2	A	376	ALA	2.7
2	A	633	GLN	2.7
2	A	561	PHE	2.7
2	A	634	ILE	2.7
2	A	669	PRO	2.7
2	A	636	SER	2.7
2	A	573	LYS	2.6
2	A	658	LYS	2.6
2	A	613	SER	2.6
2	A	610	PHE	2.6
2	A	681	GLU	2.6
2	A	137	VAL	2.6
2	A	410	HIS	2.6
2	A	674	TYR	2.6
2	A	675	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	473	ALA	2.5
2	A	407	GLU	2.5
2	A	653	ILE	2.5
2	A	331	MET	2.5
2	A	470	MET	2.5
2	A	645	LEU	2.4
2	A	625	GLU	2.4
2	A	531	LYS	2.4
2	A	448	GLN	2.4
2	A	581	ASN	2.4
2	A	641	THR	2.4
2	A	586	MET	2.4
2	A	357	GLU	2.4
2	A	583	GLY	2.3
2	A	533	LEU	2.3
2	A	468	CYS	2.3
2	A	603	PRO	2.3
2	A	431	ILE	2.3
2	A	279	GLN	2.3
2	A	519	GLY	2.3
2	A	372	SER	2.3
2	A	258	ILE	2.3
2	A	576	ILE	2.3
2	A	654	ILE	2.3
2	A	256	PRO	2.2
2	A	704	PRO	2.2
2	A	255	PRO	2.2
2	A	419	GLY	2.2
2	A	659	ILE	2.2
2	A	408	PHE	2.2
2	A	535	PRO	2.2
2	A	406	ALA	2.1
2	A	536	GLY	2.1
2	A	612	GLU	2.1
2	A	684	GLY	2.1
2	A	615	LYS	2.1
2	A	602	PRO	2.1
2	A	404	LEU	2.1
2	A	562	TRP	2.1
2	A	587	GLY	2.1
2	A	467	ILE	2.0
2	A	708	THR	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](#)

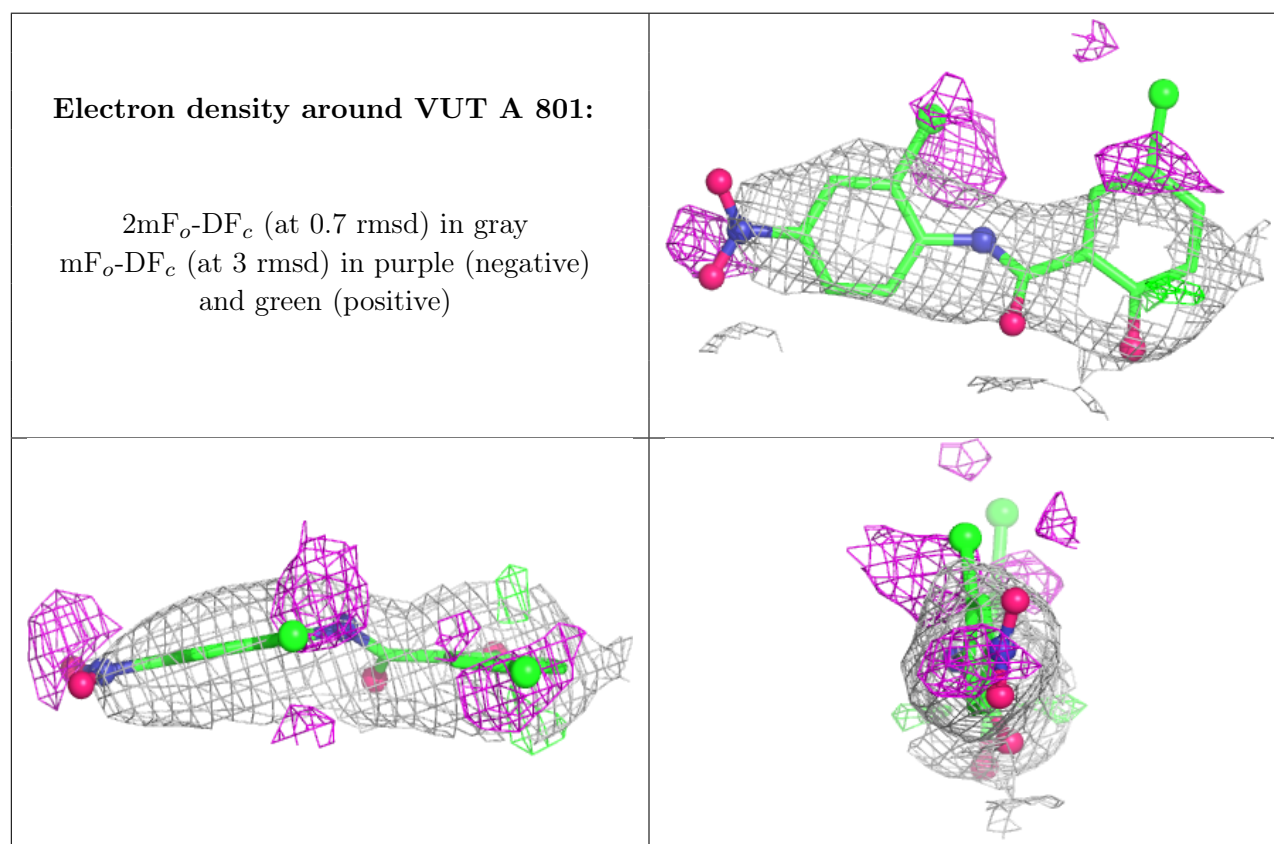
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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
3	VUT	A	801	21/21	0.82	0.19	47,110,159,212	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.