



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:21 AM BST

PDB ID : 2ZX9  
Title : alpha-L-fucosidase complexed with inhibitor, B4  
Authors : Wu, H.-J.; Ko, T.-P.; Ho, C.-W.; Lin, C.-H.; Wang, A.H.-J.  
Deposited on : 2008-12-22  
Resolution : 2.62 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.

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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 : 2.13.1  
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) : 2.13.1

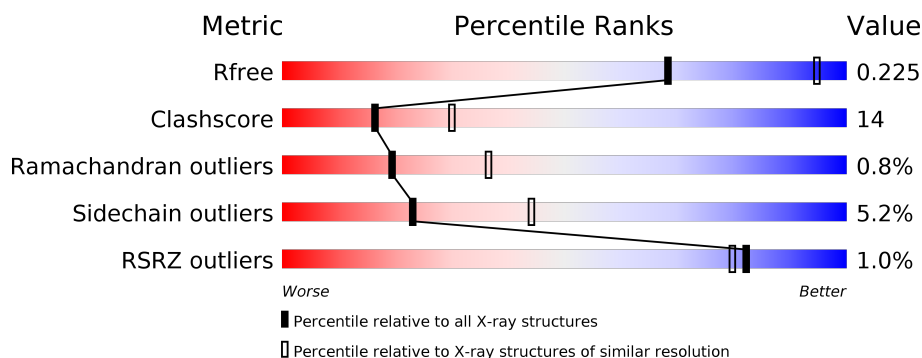
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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  $\geq 3$ , 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	A	455	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </div> </div>
1	B	455	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZX9	A	901	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7739 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.

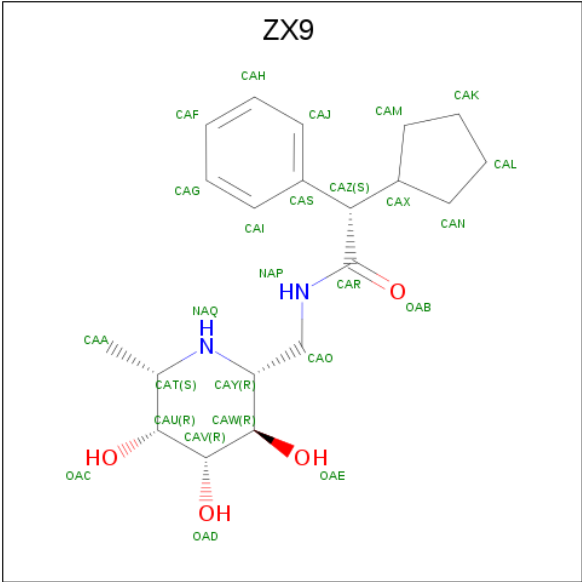
- Molecule 1 is a protein called Alpha-L-fucosidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3648	2377	600	663	8			
1	B	442	Total	C	N	O	S	0	0	0
			3648	2377	600	663	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	HIS	-	EXPRESSION TAG	UNP Q9WYE2
A	451	HIS	-	EXPRESSION TAG	UNP Q9WYE2
A	452	HIS	-	EXPRESSION TAG	UNP Q9WYE2
A	453	HIS	-	EXPRESSION TAG	UNP Q9WYE2
A	454	HIS	-	EXPRESSION TAG	UNP Q9WYE2
A	455	HIS	-	EXPRESSION TAG	UNP Q9WYE2
B	450	HIS	-	EXPRESSION TAG	UNP Q9WYE2
B	451	HIS	-	EXPRESSION TAG	UNP Q9WYE2
B	452	HIS	-	EXPRESSION TAG	UNP Q9WYE2
B	453	HIS	-	EXPRESSION TAG	UNP Q9WYE2
B	454	HIS	-	EXPRESSION TAG	UNP Q9WYE2
B	455	HIS	-	EXPRESSION TAG	UNP Q9WYE2

- Molecule 2 is (2S)-2-cyclopentyl-2-phenyl-N-{[(2R,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyl piperidin-2-yl]methyl}ethanamide (three-letter code: ZX9) (formula: C<sub>20</sub>H<sub>30</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	20	2	4		
2	B	1	Total	C	N	O	0	0
			26	20	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total	O	0	0
			191	191		
3	B	200	Total	O	0	0
			200	200		



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.81Å 180.81Å 169.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.45 – 2.62 25.45 – 2.62	Depositor EDS
% Data completeness (in resolution range)	95.3 (25.45-2.62) 95.2 (25.45-2.62)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.60Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.162 , 0.227 0.160 , 0.225	Depositor DCC
$R_{free}$ test set	1521 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZX9

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	1.01	1/3768 (0.0%)	0.97	5/5120 (0.1%)
1	B	0.99	1/3768 (0.0%)	0.98	7/5120 (0.1%)
All	All	1.00	2/7536 (0.0%)	0.98	12/10240 (0.1%)

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
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	GLU	CG-CD	5.40	1.60	1.51
1	A	76	GLU	CG-CD	5.01	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	B	179	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	179	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	B	179	ARG	CG-CD-NE	5.74	123.85	111.80
1	A	27	ALA	N-CA-C	-5.64	95.76	111.00
1	B	77	SER	N-CA-C	-5.46	96.25	111.00
1	B	148	GLY	N-CA-C	5.44	126.70	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	134	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	179	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	77	SER	N-CA-C	-5.15	97.10	111.00
1	A	195	ARG	NE-CZ-NH2	5.11	122.85	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	TYR	Sidechain
1	A	237	TYR	Sidechain
1	B	201	TYR	Sidechain

## 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	3648	0	3512	105	0
1	B	3648	0	3512	101	0
2	A	26	0	30	10	0
2	B	26	0	30	5	0
3	A	191	0	0	4	0
3	B	200	0	0	1	1
All	All	7739	0	7084	207	1

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 (207) 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:B:902:ZX9:HAJ	2:B:902:ZX9:HAN	1.23	1.09
2:A:901:ZX9:HAJ	2:A:901:ZX9:HAN	1.36	1.03
1:A:297:GLY:H	1:A:300:HIS:HD2	1.05	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LYS:NZ	1:B:439:SER:HB2	1.87	0.90
2:B:902:ZX9:HAJ	2:B:902:ZX9:CAN	2.03	0.89
1:A:399:GLU:HA	1:A:425:ASN:ND2	1.88	0.87
1:B:42:GLY:O	1:B:294:ARG:HG2	1.74	0.87
1:B:297:GLY:H	1:B:300:HIS:HD2	1.19	0.85
1:A:381:ASN:H	1:A:381:ASN:HD22	1.24	0.84
1:A:16:ARG:NH1	1:B:16:ARG:HH11	1.81	0.78
1:B:350:LYS:HZ2	1:B:439:SER:HB2	1.48	0.76
1:A:400:ASP:HA	1:A:424:LYS:O	1.84	0.76
1:B:432:LYS:HE2	1:B:436:GLU:OE1	1.87	0.75
1:A:405:ALA:HB1	1:A:447:VAL:O	1.87	0.74
1:A:16:ARG:HG2	1:B:260:TRP:CZ2	2.23	0.73
1:A:297:GLY:H	1:A:300:HIS:CD2	1.98	0.73
1:B:297:GLY:H	1:B:300:HIS:CD2	2.05	0.72
1:B:420:LYS:HG2	1:B:422:VAL:HG22	1.73	0.69
1:B:161:VAL:HG13	1:B:166:LEU:HB2	1.75	0.69
1:B:22:LYS:O	1:B:26:LYS:HG3	1.92	0.68
1:A:263:LYS:HD3	1:A:278:TYR:CE1	2.28	0.68
1:A:426:LEU:HD21	1:A:428:ILE:HD11	1.75	0.68
1:A:203:ASP:O	1:A:207:LYS:HG3	1.96	0.66
1:A:399:GLU:HA	1:A:425:ASN:HD22	1.58	0.66
1:B:134:LEU:HD13	1:B:153:LEU:HD12	1.78	0.65
1:B:92:GLU:HB2	1:B:94:GLU:OE2	1.97	0.64
1:A:381:ASN:ND2	1:A:381:ASN:H	1.95	0.64
2:A:901:ZX9:HAJ	2:A:901:ZX9:CAN	2.20	0.64
1:A:433:LYS:NZ	3:A:645:HOH:O	2.31	0.63
1:B:350:LYS:HZ3	1:B:439:SER:HB2	1.62	0.63
1:A:134:LEU:O	1:A:154:VAL:HG23	1.98	0.63
1:B:395:LYS:HE2	1:B:427:GLU:OE1	1.98	0.63
1:B:94:GLU:H	1:B:94:GLU:CD	2.02	0.63
1:A:369:GLU:HB2	1:A:397:VAL:HB	1.81	0.63
1:B:41:PRO:O	1:B:294:ARG:NH1	2.32	0.63
1:A:448:GLU:HB2	3:A:609:HOH:O	2.00	0.61
1:B:27:ALA:HB1	1:B:120:LYS:HB2	1.81	0.61
1:A:51:GLY:HA3	1:A:268:HIS:HB2	1.83	0.61
2:A:901:ZX9:CAJ	2:A:901:ZX9:HAN	2.20	0.60
1:B:413:THR:HG21	1:B:434:LEU:HD22	1.84	0.59
2:B:902:ZX9:CAJ	2:B:902:ZX9:HAN	2.14	0.59
1:A:161:VAL:HG13	1:A:166:LEU:HB2	1.85	0.59
1:A:108:GLN:NE2	1:A:108:GLN:HA	2.18	0.58
1:B:125:THR:HA	1:B:171:TYR:HB3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ARG:HH21	1:B:179:ARG:HG2	1.68	0.58
1:A:293:ASN:HB3	1:A:296:GLU:HG3	1.86	0.58
1:A:297:GLY:N	1:A:300:HIS:HD2	1.89	0.58
1:B:433:LYS:HG3	1:B:434:LEU:N	2.19	0.57
1:B:431:PRO:HD2	1:B:434:LEU:HD12	1.88	0.56
1:A:27:ALA:HB1	1:A:120:LYS:HB2	1.88	0.56
1:A:286:ILE:HG22	1:A:301:MET:CE	2.36	0.56
1:A:13:GLU:HG2	3:B:460:HOH:O	2.06	0.56
1:B:420:LYS:HG2	1:B:422:VAL:CG2	2.35	0.56
1:A:134:LEU:HB3	1:A:153:LEU:HD12	1.88	0.55
1:A:398:ILE:HD12	1:A:426:LEU:HD23	1.88	0.55
1:A:447:VAL:HG12	1:A:448:GLU:N	2.21	0.55
1:A:91:PHE:CE2	1:A:95:LYS:HB3	2.42	0.55
1:A:221:LEU:HB2	1:A:251:VAL:HG12	1.89	0.55
1:A:286:ILE:CG2	1:A:301:MET:HE3	2.37	0.55
1:B:408:VAL:HG11	1:B:428:ILE:HD13	1.88	0.55
1:B:385:VAL:HB	1:B:444:LEU:HB2	1.89	0.55
1:A:369:GLU:OE1	1:A:397:VAL:HG11	2.07	0.54
1:A:138:LYS:HG2	1:A:211:GLU:OE2	2.07	0.54
1:B:301:MET:CE	1:B:336:LEU:HB3	2.38	0.54
1:A:16:ARG:HB2	3:A:471:HOH:O	2.09	0.53
1:A:248:GLU:HA	1:A:248:GLU:OE2	2.07	0.53
1:B:388:LEU:N	1:B:388:LEU:HD23	2.23	0.53
1:B:136:GLY:HA3	1:B:145:VAL:HG21	1.90	0.53
1:B:402:ASN:HA	1:B:421:ASN:OD1	2.09	0.53
1:B:35:TRP:CZ3	1:B:153:LEU:HD13	2.44	0.53
1:A:55:MET:HB3	1:A:188:PRO:HG2	1.91	0.53
1:A:379:LYS:O	1:A:380:CYS:HB2	2.09	0.52
1:B:297:GLY:N	1:B:300:HIS:HD2	1.98	0.52
1:A:16:ARG:HG2	1:B:260:TRP:CE2	2.43	0.52
1:A:134:LEU:N	1:A:134:LEU:HD23	2.26	0.51
1:B:161:VAL:CG1	1:B:166:LEU:HB2	2.40	0.51
1:B:307:LEU:HD23	1:B:344:LEU:HB2	1.93	0.51
1:B:221:LEU:HB2	1:B:251:VAL:HG12	1.91	0.51
1:A:128:HIS:CE1	2:A:901:ZX9:OAD	2.64	0.51
1:A:447:VAL:HG12	1:A:448:GLU:H	1.76	0.50
1:B:52:LYS:HA	1:B:52:LYS:HE2	1.93	0.50
1:B:293:ASN:HB3	1:B:296:GLU:HG3	1.93	0.50
1:A:233:GLU:OE1	1:A:236:LYS:HE2	2.11	0.50
1:A:145:VAL:O	1:A:150:LYS:HA	2.12	0.50
1:A:34:HIS:CG	1:A:290:PHE:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:CB	1:B:94:GLU:OE2	2.59	0.49
1:A:125:THR:HA	1:A:171:TYR:HB3	1.94	0.49
1:B:351:TYR:OH	1:B:438:ASP:HA	2.13	0.49
1:B:361:TRP:CE2	1:B:383:ILE:HD13	2.48	0.49
1:B:369:GLU:OE1	1:B:397:VAL:HG11	2.13	0.49
1:B:52:LYS:HG2	1:B:268:HIS:CD2	2.47	0.49
1:B:203:ASP:O	1:B:207:LYS:HG3	2.13	0.48
1:A:121:TYR:HA	1:A:167:ARG:O	2.13	0.48
1:A:296:GLU:HA	1:A:300:HIS:CD2	2.47	0.48
1:A:290:PHE:CD2	2:A:901:ZX9:HAA	2.48	0.48
1:A:409:ARG:HH22	1:A:416:ARG:HH11	1.62	0.48
1:B:409:ARG:NH1	1:B:414:GLY:O	2.47	0.48
1:B:398:ILE:HG21	1:B:401:LEU:HD23	1.96	0.48
1:B:404:SER:O	1:B:405:ALA:O	2.32	0.48
1:A:275:LEU:HD23	1:A:317:LYS:HA	1.94	0.48
1:A:286:ILE:CG2	1:A:301:MET:CE	2.91	0.48
1:B:301:MET:HE1	1:B:336:LEU:HB3	1.95	0.48
1:A:286:ILE:HG22	1:A:301:MET:HE2	1.95	0.47
1:A:290:PHE:HA	1:A:324:ASN:ND2	2.29	0.47
1:B:410:HIS:HB2	1:B:417:LEU:HD21	1.96	0.47
1:A:134:LEU:HD13	1:A:153:LEU:HD12	1.97	0.47
1:A:435:LEU:CD2	1:A:442:LEU:HD22	2.44	0.47
1:A:411:PHE:HB3	1:A:443:VAL:O	2.13	0.47
1:B:394:GLU:O	1:B:429:THR:HA	2.14	0.47
1:A:20:VAL:HG13	1:A:20:VAL:O	2.14	0.47
1:A:12:TRP:CZ2	1:A:236:LYS:HG3	2.50	0.47
1:A:279:LYS:HD2	1:A:280:TRP:H	1.78	0.47
1:B:106:ASP:OD2	1:B:109:GLU:HG3	2.14	0.47
1:A:73:ARG:HB2	1:A:184:PRO:HB3	1.96	0.47
1:A:304:VAL:O	1:A:308:VAL:HG23	2.15	0.47
1:B:106:ASP:CG	1:B:109:GLU:HG3	2.35	0.47
1:B:19:THR:O	1:B:20:VAL:C	2.53	0.47
1:B:301:MET:CE	1:B:340:ARG:HD2	2.45	0.46
1:B:358:THR:HG22	1:B:379:LYS:HD2	1.97	0.46
1:A:105:TRP:CZ2	1:A:107:PRO:HB3	2.51	0.46
1:A:106:ASP:OD2	1:A:109:GLU:HG3	2.16	0.46
1:A:16:ARG:NH1	1:B:16:ARG:NH1	2.59	0.46
1:A:350:LYS:HE2	1:A:351:TYR:CE2	2.50	0.46
1:B:136:GLY:CA	1:B:145:VAL:HG21	2.45	0.46
1:B:292:TYR:HB2	1:B:326:GLY:O	2.16	0.46
1:A:171:TYR:CD2	1:A:171:TYR:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:O	1:A:294:ARG:NH1	2.45	0.46
1:B:135:TRP:CE2	1:B:137:THR:HB	2.51	0.46
1:B:40:VAL:O	1:B:41:PRO:C	2.52	0.46
1:A:311:LEU:HD21	1:A:348:LEU:HD21	1.98	0.45
1:A:49:GLU:HA	3:A:551:HOH:O	2.16	0.45
1:A:108:GLN:NE2	1:A:108:GLN:CA	2.80	0.45
1:A:55:MET:HB3	1:A:188:PRO:CG	2.46	0.45
1:B:199:TYR:CZ	1:B:230:LYS:HE2	2.52	0.45
1:B:128:HIS:CE1	2:B:902:ZX9:OAD	2.70	0.45
1:B:34:HIS:CG	1:B:290:PHE:HB3	2.52	0.45
1:A:106:ASP:CG	1:A:109:GLU:HG3	2.36	0.45
1:A:16:ARG:HH12	1:B:16:ARG:HG3	1.82	0.45
1:A:351:TYR:CD1	1:A:443:VAL:HG21	2.52	0.45
1:B:410:HIS:CE1	1:B:413:THR:HG23	2.51	0.45
1:A:286:ILE:HG22	1:A:301:MET:HE3	1.98	0.44
1:A:55:MET:CE	2:A:901:ZX9:HAKA	2.47	0.44
1:A:260:TRP:CZ2	1:B:16:ARG:HG2	2.52	0.44
1:B:364:CYS:O	1:B:375:ARG:HA	2.17	0.44
1:A:402:ASN:HD22	1:A:402:ASN:HA	1.55	0.44
1:B:285:GLY:HA2	1:B:324:ASN:HB3	1.99	0.44
1:B:305:GLU:HG3	1:B:440:ILE:HG23	2.00	0.44
1:A:50:LEU:HD11	2:A:901:ZX9:CAM	2.47	0.44
1:B:351:TYR:CE1	1:B:412:LEU:HD13	2.53	0.44
1:B:434:LEU:C	1:B:436:GLU:N	2.70	0.44
1:A:108:GLN:HE21	1:A:108:GLN:CA	2.31	0.44
1:B:432:LYS:O	1:B:436:GLU:HB2	2.17	0.44
1:A:231:GLY:O	1:A:234:ASP:HB2	2.18	0.43
1:A:286:ILE:CG2	1:A:340:ARG:HD3	2.47	0.43
1:B:354:ALA:HA	1:B:384:PHE:CE1	2.53	0.43
1:A:280:TRP:CZ3	1:A:282:PHE:HB2	2.52	0.43
1:B:301:MET:HE2	1:B:340:ARG:HD2	2.00	0.43
1:B:7:ARG:HA	1:B:7:ARG:HD2	1.82	0.43
1:A:301:MET:HE2	1:A:301:MET:HB3	1.61	0.43
1:A:217:LEU:HD11	1:A:246:HIS:HB2	2.00	0.43
1:B:303:SER:O	1:B:304:VAL:C	2.56	0.43
1:A:398:ILE:HD12	1:A:426:LEU:CD2	2.48	0.43
1:A:50:LEU:HD11	2:A:901:ZX9:HAM	2.01	0.43
1:B:106:ASP:HB3	1:B:109:GLU:HG3	1.99	0.43
1:B:29:PHE:CD1	1:B:119:ALA:HA	2.54	0.43
1:B:123:ILE:HG23	1:B:169:GLY:C	2.39	0.43
1:B:325:VAL:O	1:B:327:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:VAL:O	1:B:270:ASN:HB2	2.19	0.42
1:B:434:LEU:O	1:B:435:LEU:C	2.55	0.42
1:A:106:ASP:HB3	1:A:109:GLU:HG3	2.01	0.42
1:A:381:ASN:ND2	1:A:381:ASN:N	2.65	0.42
1:B:12:TRP:CZ2	1:B:236:LYS:HG3	2.54	0.42
1:B:77:SER:O	1:B:78:PRO:C	2.54	0.42
1:A:120:LYS:HD3	1:A:120:LYS:HA	1.90	0.42
1:B:177:ASP:OD1	1:B:179:ARG:HB2	2.20	0.42
1:A:32:PHE:HB3	1:A:324:ASN:HA	2.01	0.42
1:A:407:THR:O	1:A:407:THR:HG23	2.20	0.42
1:A:290:PHE:CE2	2:A:901:ZX9:HAA	2.54	0.42
1:B:430:VAL:HG12	1:B:435:LEU:HG	2.02	0.42
1:A:55:MET:HE2	2:A:901:ZX9:HAKA	2.01	0.42
1:B:361:TRP:NE1	1:B:383:ILE:HD13	2.35	0.42
1:A:121:TYR:HB3	1:A:167:ARG:HB2	2.02	0.42
1:A:148:GLY:HA3	1:A:149:PRO:HD3	1.81	0.41
1:B:297:GLY:HA3	1:B:299:GLU:OE1	2.20	0.41
1:A:311:LEU:CD2	1:A:348:LEU:HD21	2.50	0.41
1:B:235:LEU:HD12	1:B:257:VAL:HG11	2.03	0.41
1:A:292:TYR:HB2	1:A:326:GLY:O	2.19	0.41
1:A:431:PRO:HD2	1:A:434:LEU:HD12	2.02	0.41
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.92	0.41
1:B:307:LEU:HD12	1:B:307:LEU:HA	1.80	0.41
1:B:31:ILE:HG23	1:B:325:VAL:HG13	2.03	0.41
2:B:902:ZX9:CAJ	2:B:902:ZX9:CAN	2.78	0.41
1:A:280:TRP:O	1:A:319:GLY:HA2	2.21	0.41
1:B:216:TYR:O	1:B:217:LEU:C	2.59	0.41
1:B:312:VAL:HG11	1:B:386:ILE:HG21	2.02	0.41
1:B:301:MET:HE1	1:B:340:ARG:NH1	2.35	0.41
1:A:369:GLU:HA	1:A:399:GLU:OE1	2.21	0.40
1:B:395:LYS:CE	1:B:427:GLU:OE1	2.68	0.40
1:B:80:TRP:CH2	1:B:84:VAL:HG21	2.56	0.40
1:B:312:VAL:HG11	1:B:386:ILE:CG2	2.51	0.40
1:A:196:PRO:O	1:A:197:ASN:HB2	2.22	0.40
1:A:21:PRO:HB3	1:A:248:GLU:OE2	2.22	0.40
1:A:381:ASN:O	1:A:383:ILE:HD12	2.21	0.40
1:B:279:LYS:HD2	1:B:279:LYS:HA	1.90	0.40
1:A:341:LEU:HA	1:A:341:LEU:HD23	1.95	0.40
1:B:31:ILE:HG12	1:B:119:ALA:HB2	2.03	0.40
1:B:400:ASP:HA	1:B:424:LYS:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:HOH:O	3:B:602:HOH:O[3_555]	1.63	0.57

## 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	440/455 (97%)	411 (93%)	25 (6%)	4 (1%)	17	33
1	B	440/455 (97%)	405 (92%)	32 (7%)	3 (1%)	22	41
All	All	880/910 (97%)	816 (93%)	57 (6%)	7 (1%)	19	36

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	ALA
1	B	405	ALA
1	B	148	GLY
1	A	406	GLY
1	A	258	PRO
1	B	304	VAL
1	A	148	GLY

### 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	382/395 (97%)	364 (95%)	18 (5%)	26	49
1	B	382/395 (97%)	360 (94%)	22 (6%)	20	38
All	All	764/790 (97%)	724 (95%)	40 (5%)	23	44

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	16	ARG
1	A	19	THR
1	A	32	PHE
1	A	66	GLU
1	A	76	GLU
1	A	108	GLN
1	A	112	ASP
1	A	134	LEU
1	A	294	ARG
1	A	299	GLU
1	A	346	GLU
1	A	381	ASN
1	A	397	VAL
1	A	402	ASN
1	A	415	GLU
1	A	426	LEU
1	A	432	LYS
1	B	19	THR
1	B	22	LYS
1	B	26	LYS
1	B	32	PHE
1	B	37	ILE
1	B	66	GLU
1	B	76	GLU
1	B	92	GLU
1	B	134	LEU
1	B	159	LYS
1	B	179	ARG
1	B	222	TRP
1	B	263	LYS
1	B	299	GLU
1	B	325	VAL
1	B	353	ASP
1	B	381	ASN

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Mol	Chain	Res	Type
1	B	392	THR
1	B	402	ASN
1	B	407	THR
1	B	436	GLU
1	B	437	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	108	GLN
1	A	300	HIS
1	A	381	ASN
1	A	402	ASN
1	A	425	ASN
1	B	300	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 monosaccharides 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	ZX9	B	902	-	27,28,28	0.49	0	34,39,39	1.44	6 (17%)
2	ZX9	A	901	-	27,28,28	0.50	0	34,39,39	1.33	5 (14%)

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	ZX9	B	902	-	-	10/17/44/44	0/3/3/3
2	ZX9	A	901	-	-	13/17/44/44	0/3/3/3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	ZX9	CAY-CAO-NAP	-4.23	103.19	112.78
2	A	901	ZX9	CAY-CAO-NAP	-3.16	105.62	112.78
2	A	901	ZX9	CAK-CAM-CAX	-3.14	96.26	104.96
2	B	902	ZX9	CAL-CAN-CAX	-2.76	97.31	104.96
2	A	901	ZX9	CAI-CAS-CAZ	-2.75	116.43	120.85
2	B	902	ZX9	CAT-NAQ-CAY	-2.73	108.78	113.21
2	A	901	ZX9	CAT-NAQ-CAY	-2.70	108.83	113.21
2	B	902	ZX9	CAZ-CAR-NAP	-2.43	111.78	115.70
2	B	902	ZX9	CAV-CAW-CAY	-2.29	107.66	111.02
2	B	902	ZX9	CAJ-CAS-CAI	2.13	120.94	118.29
2	A	901	ZX9	CAV-CAW-CAY	-2.01	108.07	111.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	902	ZX9	CAM-CAX-CAZ-CAS
2	B	902	ZX9	CAM-CAX-CAZ-CAR
2	B	902	ZX9	CAN-CAX-CAZ-CAR
2	B	902	ZX9	NAP-CAO-CAY-NAQ
2	B	902	ZX9	NAP-CAO-CAY-CAW
2	A	901	ZX9	CAM-CAX-CAZ-CAS
2	A	901	ZX9	CAM-CAX-CAZ-CAR
2	A	901	ZX9	CAN-CAX-CAZ-CAR

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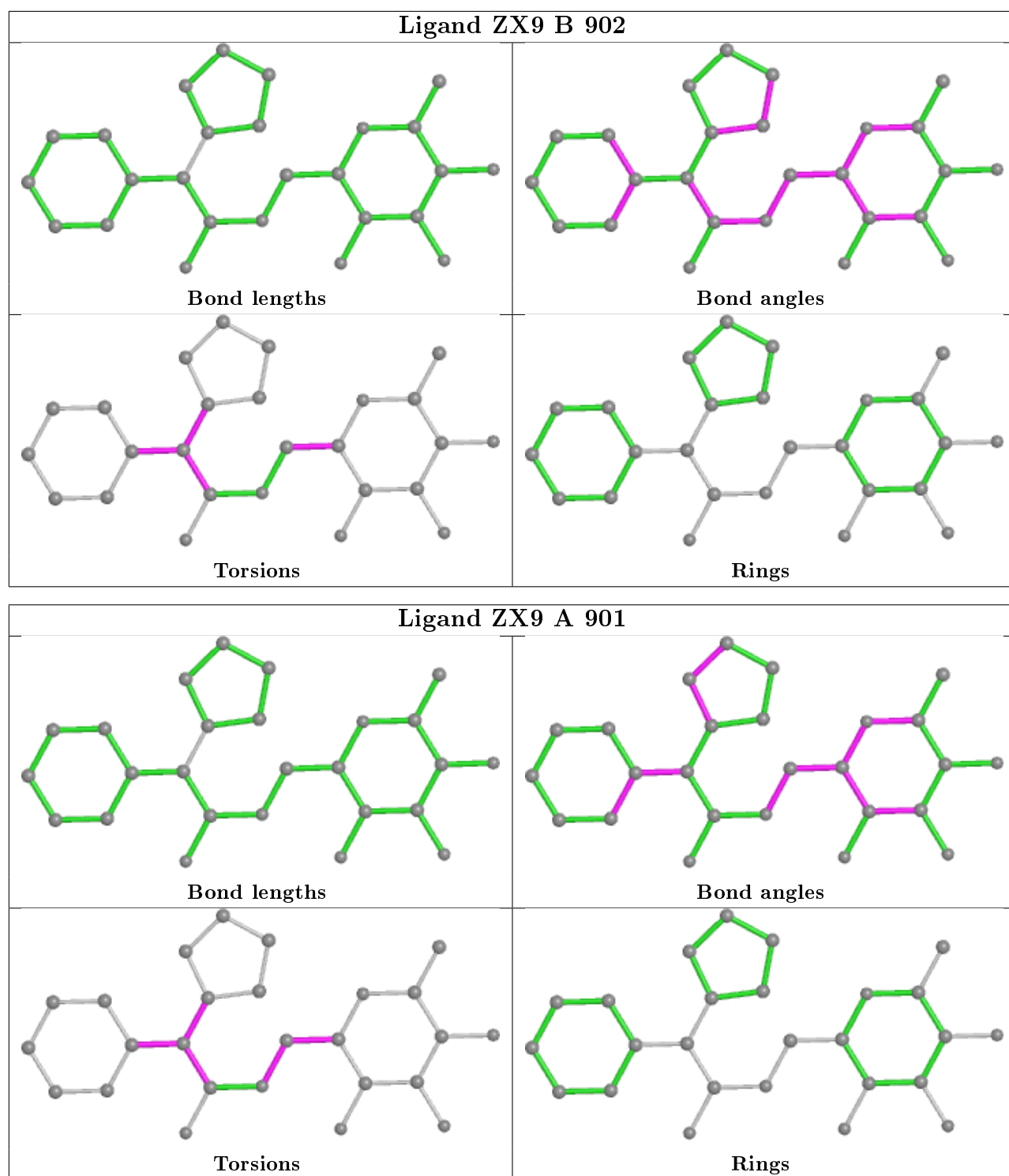
Mol	Chain	Res	Type	Atoms
2	A	901	ZX9	OAB-CAR-CAZ-CAX
2	A	901	ZX9	NAP-CAO-CAY-NAQ
2	A	901	ZX9	NAP-CAO-CAY-CAW
2	A	901	ZX9	CAI-CAS-CAZ-CAX
2	A	901	ZX9	CAJ-CAS-CAZ-CAX
2	B	902	ZX9	OAB-CAR-CAZ-CAS
2	A	901	ZX9	OAB-CAR-CAZ-CAS
2	B	902	ZX9	CAI-CAS-CAZ-CAX
2	B	902	ZX9	CAJ-CAS-CAZ-CAX
2	A	901	ZX9	NAP-CAR-CAZ-CAX
2	A	901	ZX9	CAN-CAX-CAZ-CAS
2	B	902	ZX9	NAP-CAR-CAZ-CAS
2	A	901	ZX9	NAP-CAR-CAZ-CAS
2	A	901	ZX9	CAY-CAO-NAP-CAR
2	B	902	ZX9	NAP-CAR-CAZ-CAX

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	ZX9	5	0
2	A	901	ZX9	10	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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	A	442/455 (97%)	-0.60	4 (0%) 84 82	18, 34, 60, 91	0
1	B	442/455 (97%)	-0.52	5 (1%) 80 78	20, 36, 61, 75	0
All	All	884/910 (97%)	-0.56	9 (1%) 82 80	18, 35, 61, 91	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	448	GLU	3.8
1	B	406	GLY	2.8
1	B	385	VAL	2.7
1	A	385	VAL	2.5
1	A	392	THR	2.5
1	A	404	SER	2.4
1	B	22	LYS	2.4
1	B	386	ILE	2.4
1	B	273	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 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,

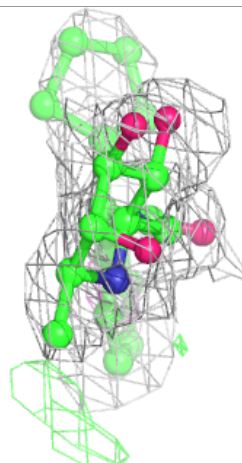
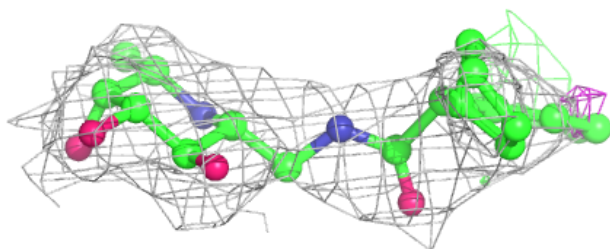
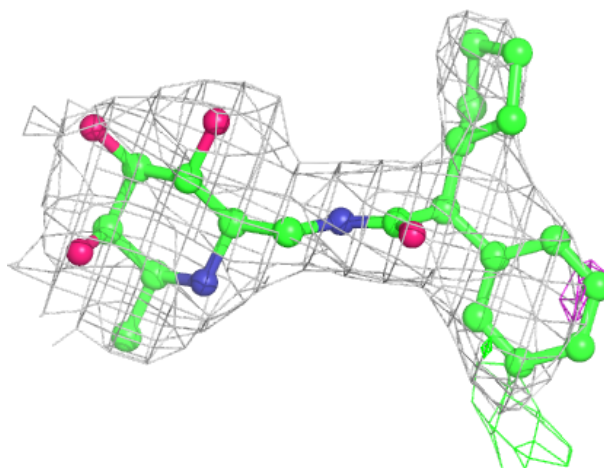
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZX9	A	901	26/26	0.84	0.23	29,48,57,58	0
2	ZX9	B	902	26/26	0.88	0.18	27,48,58,58	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.

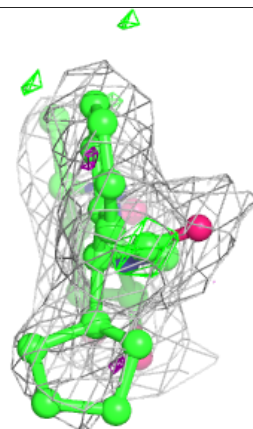
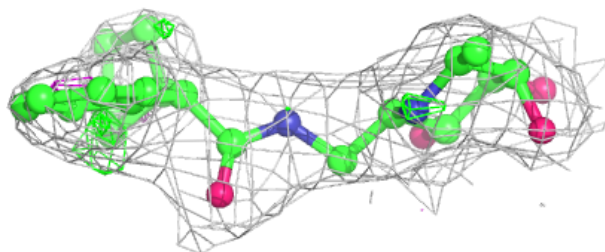
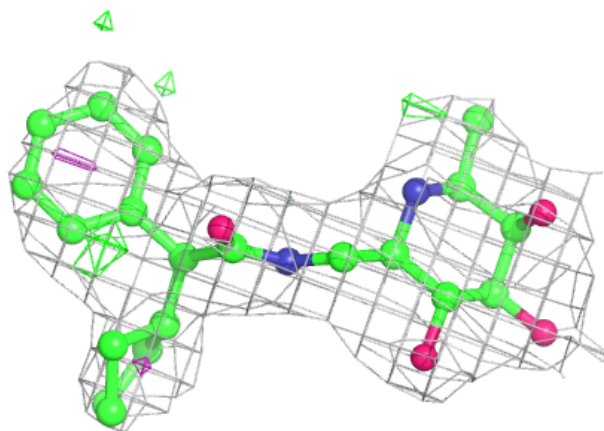
**Electron density around ZX9 A 901:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZX9 B 902:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.