



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2020 – 10:40 AM EST

PDB ID : 6VC9  
Title : TB19 complex  
Authors : Zhou, Y.F.; Lord, D.M.  
Deposited on : 2019-12-20  
Resolution : 2.25 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:

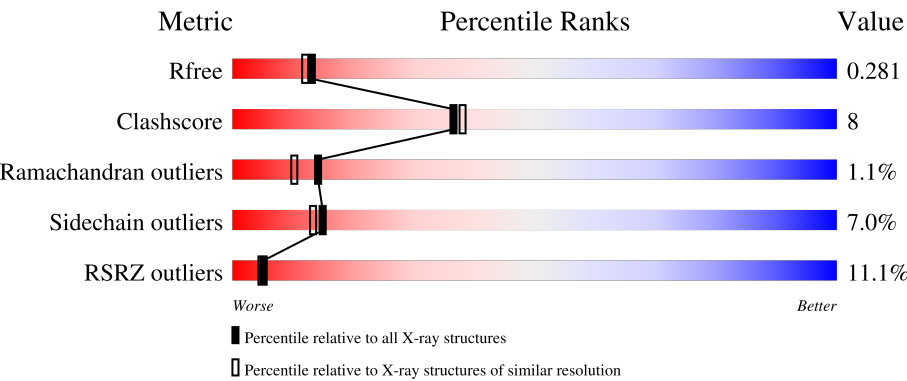
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	H	233	<div><div>16%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>27%18%<span>••</span>49%</div></div>
2	L	215	<div><div>13%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>28%19%<span>•</span>50%</div></div>
3	A	529	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>87%11%<span>••</span></div></div>
4	B	5	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%40%20%</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
8	EDO	A	612	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6035 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 TB19 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	118	Total	C	N	O	S	0	0	0
			899	559	155	182	3			

- Molecule 2 is a protein called TB19 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	108	Total	C	N	O	S	0	0	0
			841	533	137	168	3			

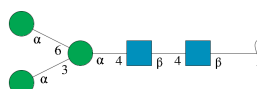
- Molecule 3 is a protein called 5'-nucleotidase, ecto (CD73), isoform CRA\_a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	523	Total	C	N	O	S	0	0	0
			4074	2590	698	768	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	550	HIS	-	expression tag	UNP Q53Z63
A	551	HIS	-	expression tag	UNP Q53Z63
A	552	HIS	-	expression tag	UNP Q53Z63
A	553	HIS	-	expression tag	UNP Q53Z63
A	554	HIS	-	expression tag	UNP Q53Z63
A	555	HIS	-	expression tag	UNP Q53Z63

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

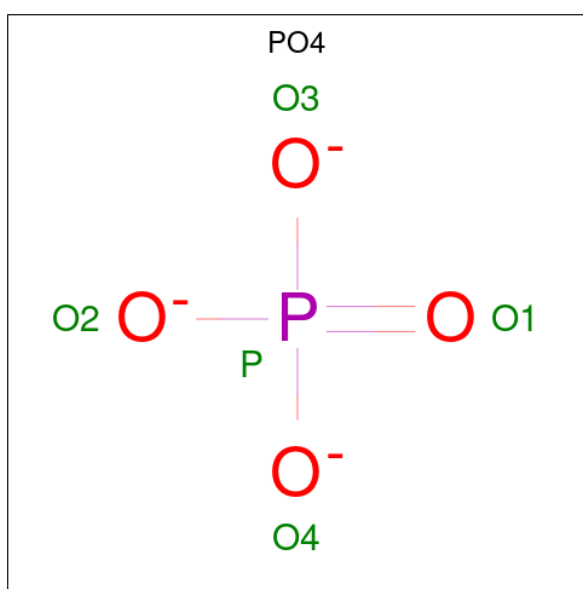


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

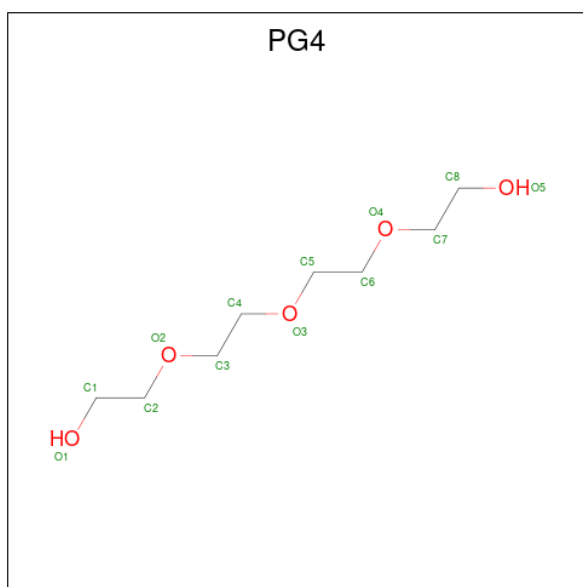
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



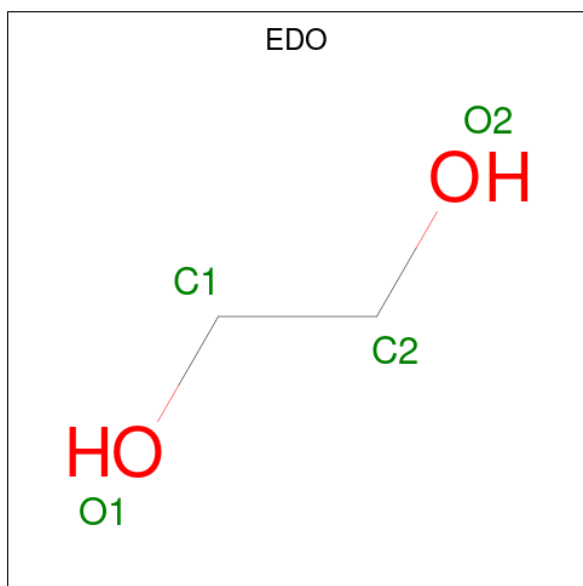
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	A	1	Total	O	P	0	0
			5	4	1		
6	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



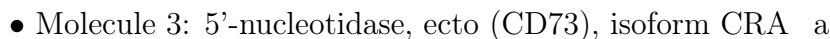
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

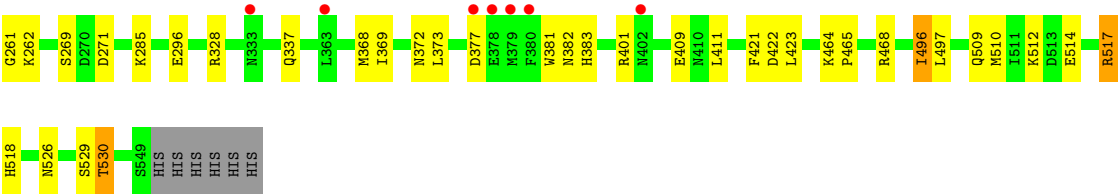
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	9	Total 9	O 9	0	0
9	L	15	Total 15	O 15	0	0
9	A	102	Total 102	O 102	0	0

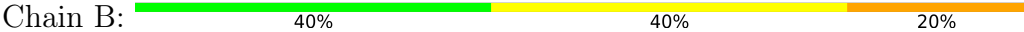


- Molecule 1: TB19 heavy chain





● Molecule 4:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.31Å 74.22Å 148.33Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25 29.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.25) 99.6 (29.87-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.237 , 0.279 0.245 , 0.281	Depositor DCC
$R_{free}$ test set	2017 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: ZN, NAG, PO4, EDO, PG4, MAN

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	H	2.26	10/916 (1.1%)	1.03	2/1245 (0.2%)
2	L	1.51	9/862 (1.0%)	1.06	3/1174 (0.3%)
3	A	0.83	2/4160 (0.0%)	0.91	1/5636 (0.0%)
All	All	1.27	21/5938 (0.4%)	0.95	6/8055 (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	H	0	2
2	L	0	2
All	All	0	4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	6	GLU	CD-OE2	54.11	1.85	1.25
2	L	106	GLU	CD-OE1	21.20	1.49	1.25
2	L	106	GLU	CD-OE2	18.38	1.45	1.25
1	H	119	SER	C-O	14.73	1.51	1.23
1	H	7	SER	CB-OG	12.79	1.58	1.42
1	H	6	GLU	CD-OE1	12.63	1.39	1.25
2	L	106	GLU	C-O	8.98	1.40	1.23
1	H	10	GLY	C-O	8.85	1.37	1.23
3	A	125	GLU	CD-OE2	7.97	1.34	1.25
3	A	125	GLU	CD-OE1	7.10	1.33	1.25
1	H	56	THR	C-O	7.04	1.36	1.23
2	L	86	ILE	C-O	6.74	1.36	1.23
1	H	32	ASN	C-O	6.29	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	6	GLN	CD-NE2	6.20	1.48	1.32
1	H	72	ASP	CG-OD2	6.13	1.39	1.25
2	L	78	SER	C-O	5.97	1.34	1.23
1	H	62	SER	CB-OG	5.60	1.49	1.42
2	L	46	ARG	C-O	5.46	1.33	1.23
2	L	38	GLN	C-N	5.31	1.46	1.34
2	L	38	GLN	C-O	5.28	1.33	1.23
1	H	50	ARG	C-O	5.08	1.32	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	106	GLU	OE1-CD-OE2	10.52	135.93	123.30
1	H	6	GLU	OE1-CD-OE2	8.52	133.52	123.30
2	L	83	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	H	6	GLU	CG-CD-OE2	-6.36	105.58	118.30
3	A	296	GLU	CB-CA-C	-6.26	97.88	110.40
2	L	83	ASP	CB-CG-OD2	-5.34	113.49	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	6	GLU	Sidechain
1	H	91	ALA	Mainchain
2	L	45	PRO	Mainchain
2	L	50	TYR	Peptide

## 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	H	899	0	880	34	0
2	L	841	0	811	24	0
3	A	4074	0	4046	37	0
4	B	61	0	52	1	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	15	0	0	0	0
7	A	13	0	18	5	0
8	A	4	0	6	4	0
9	A	102	0	0	8	0
9	H	9	0	0	0	0
9	L	15	0	0	2	0
All	All	6035	0	5813	93	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 8.

All (93) 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:H:6:GLU:CD	1:H:6:GLU:OE2	1.85	1.15
3:A:381:TRP:O	9:A:701:HOH:O	1.74	1.04
3:A:101:VAL:HG22	8:A:612:EDO:H11	1.44	0.98
1:H:22:CYS:O	1:H:77:GLN:HB2	1.64	0.96
3:A:101:VAL:HG22	8:A:612:EDO:C1	2.10	0.81
1:H:35:ASN:HD22	1:H:47:TRP:HE1	1.31	0.79
3:A:381:TRP:C	9:A:701:HOH:O	2.18	0.78
2:L:56:ALA:HB3	2:L:59:ILE:HD13	1.69	0.75
1:H:71:ILE:HG12	1:H:78:PHE:HB3	1.73	0.71
3:A:256:LYS:NZ	3:A:257:GLU:OE2	2.18	0.71
1:H:109:TRP:HB2	2:L:44:THR:CG2	2.23	0.68
3:A:129:GLU:OE1	3:A:129:GLU:O	2.12	0.67
3:A:269:SER:OG	3:A:271:ASP:OD1	2.08	0.66
1:H:5:GLN:HA	1:H:5:GLN:OE1	1.98	0.63
2:L:36:TRP:CE2	2:L:74:LEU:HB2	2.35	0.62
3:A:526:ASN:O	3:A:530:THR:HG23	2.01	0.60
3:A:373:LEU:HA	3:A:382:ASN:HD21	1.67	0.60
3:A:58:MET:HE3	3:A:285:LYS:HG3	1.83	0.59
1:H:18:LEU:O	1:H:81:LYS:HA	2.01	0.59
3:A:223:PHE:N	9:A:702:HOH:O	2.36	0.59
2:L:10:THR:HA	2:L:104:TYR:O	2.02	0.59
1:H:86:THR:O	1:H:117:VAL:HG21	2.04	0.58
2:L:27:GLN:NE2	9:A:706:HOH:O	2.37	0.57
3:A:251:GLY:H	7:A:611:PG4:H51	1.69	0.57
1:H:71:ILE:HG12	1:H:78:PHE:CB	2.36	0.56
1:H:29:ILE:HD12	1:H:76:ASN:OD1	2.06	0.55
1:H:17:THR:O	1:H:18:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:GLY:HA3	1:H:69:MET:HE3	1.88	0.55
3:A:75:GLU:CD	9:A:705:HOH:O	2.45	0.55
1:H:29:ILE:CD1	1:H:76:ASN:OD1	2.55	0.55
2:L:50:TYR:C	2:L:51:GLY:O	2.44	0.55
3:A:175:GLY:HA2	3:A:218:LEU:O	2.08	0.54
2:L:34:PHE:O	2:L:51:GLY:O	2.24	0.54
1:H:11:LEU:HD23	1:H:11:LEU:O	2.07	0.54
3:A:337:GLN:HA	3:A:337:GLN:OE1	2.09	0.53
1:H:2:GLU:HA	1:H:26:GLY:HA3	1.89	0.53
2:L:21:LEU:HB3	9:L:312:HOH:O	2.08	0.53
3:A:422:ASP:OD2	3:A:518:HIS:NE2	2.41	0.53
1:H:6:GLU:OE1	1:H:6:GLU:N	2.43	0.52
1:H:3:GLN:CD	1:H:3:GLN:O	2.48	0.51
2:L:66:SER:HB3	2:L:73:THR:OG1	2.11	0.51
2:L:79:LEU:HD12	2:L:107:ILE:HG22	1.93	0.50
2:L:34:PHE:CE2	2:L:72:PHE:CD1	3.00	0.50
3:A:75:GLU:HG3	9:A:705:HOH:O	2.12	0.50
1:H:68:THR:OG1	1:H:81:LYS:HB2	2.12	0.49
1:H:87:ALA:O	1:H:90:THR:HG22	2.12	0.49
3:A:262:LYS:HE2	7:A:611:PG4:O4	2.12	0.49
3:A:368:MET:HG2	3:A:421:PHE:CD2	2.48	0.49
2:L:56:ALA:HB1	9:L:314:HOH:O	2.11	0.49
1:H:10:GLY:O	1:H:116:THR:HG22	2.12	0.49
3:A:261:GLY:HA2	7:A:611:PG4:H21	1.95	0.49
2:L:13:LEU:O	2:L:13:LEU:HD23	2.12	0.49
3:A:57:CYS:O	3:A:58:MET:HG2	2.12	0.48
1:H:49:GLY:HA3	1:H:69:MET:CE	2.44	0.48
2:L:12:SER:HA	2:L:106:GLU:O	2.12	0.48
3:A:231:GLN:HA	3:A:269:SER:HA	1.95	0.47
3:A:251:GLY:H	7:A:611:PG4:C5	2.27	0.47
1:H:4:LEU:HA	1:H:23:THR:O	2.14	0.47
3:A:422:ASP:O	3:A:496:ILE:HA	2.15	0.47
2:L:13:LEU:C	2:L:13:LEU:HD23	2.35	0.47
3:A:510:MET:O	3:A:514:GLU:HB2	2.14	0.47
1:H:61:PRO:HA	1:H:64:LYS:HB2	1.96	0.46
3:A:372:ASN:O	3:A:383:HIS:NE2	2.49	0.45
3:A:517:ARG:HG2	3:A:517:ARG:HH11	1.82	0.45
1:H:72:ASP:CG	1:H:75:LYS:HB2	2.36	0.45
9:A:703:HOH:O	4:B:4:MAN:O3	2.21	0.45
1:H:29:ILE:HG12	1:H:29:ILE:O	2.16	0.45
3:A:39:SER:HA	8:A:612:EDO:C2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:79:LEU:HD13	2:L:80:GLN:N	2.32	0.44
1:H:3:GLN:NE2	1:H:25:SER:OG	2.47	0.44
3:A:181:THR:N	3:A:182:PRO:CD	2.80	0.44
1:H:6:GLU:OE2	1:H:94:TYR:HA	2.17	0.44
2:L:95:LEU:HA	2:L:96:PRO:C	2.38	0.44
3:A:75:GLU:CG	9:A:705:HOH:O	2.65	0.43
1:H:29:ILE:N	1:H:29:ILE:HD13	2.32	0.43
3:A:251:GLY:H	7:A:611:PG4:C6	2.31	0.43
2:L:33:TYR:O	2:L:91:GLN:HA	2.18	0.43
3:A:369:ILE:HG13	3:A:496:ILE:HD11	2.01	0.42
1:H:47:TRP:CZ3	2:L:96:PRO:HA	2.55	0.42
1:H:38:ARG:HG2	1:H:48:ILE:HD11	2.01	0.42
2:L:56:ALA:HB3	2:L:59:ILE:CD1	2.45	0.42
1:H:51:ILE:HA	1:H:56:THR:O	2.19	0.42
3:A:465:PRO:HA	3:A:468:ARG:HD2	2.02	0.42
1:H:3:GLN:C	1:H:3:GLN:CD	2.78	0.42
2:L:97:TYR:OH	3:A:189:THR:HG22	2.20	0.41
3:A:38:HIS:CE1	3:A:85:ASP:HB3	2.56	0.41
2:L:79:LEU:CD1	2:L:107:ILE:HG22	2.50	0.41
2:L:35:SER:HB2	2:L:49:ILE:O	2.20	0.41
3:A:129:GLU:HB3	3:A:130:PRO:HD3	2.03	0.41
2:L:18:ARG:HG3	2:L:77:SER:HA	2.02	0.41
3:A:101:VAL:CG2	8:A:612:EDO:H22	2.52	0.40
1:H:4:LEU:CD2	1:H:24:VAL:HB	2.51	0.40
1:H:4:LEU:HD22	1:H:24:VAL:HB	2.03	0.40

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	H	116/233 (50%)	101 (87%)	11 (10%)	4 (3%)	<b>3</b> <b>1</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	106/215 (49%)	98 (92%)	6 (6%)	2 (2%)	8	4
3	A	521/529 (98%)	492 (94%)	27 (5%)	2 (0%)	34	37
All	All	743/977 (76%)	691 (93%)	44 (6%)	8 (1%)	14	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	18	LEU
1	H	76	ASN
1	H	29	ILE
1	H	118	SER
2	L	51	GLY
3	A	130	PRO
2	L	41	PRO
3	A	88	GLN

### 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	H	102/203 (50%)	90 (88%)	12 (12%)	5	3
2	L	94/190 (50%)	82 (87%)	12 (13%)	4	2
3	A	448/456 (98%)	427 (95%)	21 (5%)	26	29
All	All	644/849 (76%)	599 (93%)	45 (7%)	15	13

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	GLN
1	H	28	SER
1	H	29	ILE
1	H	62	SER
1	H	70	SER
1	H	71	ILE

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Mol	Chain	Res	Type
1	H	82	LEU
1	H	85	VAL
1	H	92	ILE
1	H	105	SER
1	H	114	LEU
1	H	117	VAL
2	L	5	THR
2	L	9	THR
2	L	10	THR
2	L	11	LEU
2	L	13	LEU
2	L	22	SER
2	L	64	SER
2	L	70	THR
2	L	77	SER
2	L	84	PHE
2	L	90	GLN
2	L	101	GLN
3	A	47	ASP
3	A	49	SER
3	A	75	GLU
3	A	129	GLU
3	A	173	ILE
3	A	180	GLU
3	A	206	LYS
3	A	328	ARG
3	A	377	ASP
3	A	401	ARG
3	A	409	GLU
3	A	411	LEU
3	A	423	LEU
3	A	464	LYS
3	A	496	ILE
3	A	497	LEU
3	A	509	GLN
3	A	512	LYS
3	A	517	ARG
3	A	529	SER
3	A	530	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	31	ASN
1	H	35	ASN
1	H	108	ASN
2	L	90	GLN
2	L	101	GLN
3	A	351	GLN
3	A	382	ASN
3	A	410	ASN
3	A	526	ASN

### 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 ⓘ

5 monosaccharides 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	$\# Z  > 2$
4	NAG	B	1	3,4	14,14,15	0.42	0	17,19,21	0.74	0
4	NAG	B	2	4	14,14,15	0.33	0	17,19,21	1.09	1 (5%)
4	MAN	B	3	4	11,11,12	0.49	0	15,15,17	1.45	3 (20%)
4	MAN	B	4	4	11,11,12	0.76	0	15,15,17	1.74	4 (26%)
4	MAN	B	5	4	11,11,12	0.47	0	15,15,17	0.67	0

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
4	NAG	B	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	MAN	B	3	4	-	2/2/19/22	0/1/1/1
4	MAN	B	4	4	-	2/2/19/22	0/1/1/1
4	MAN	B	5	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4	MAN	C1-C2-C3	4.34	115.00	109.67
4	B	3	MAN	C1-C2-C3	3.41	113.86	109.67
4	B	4	MAN	C2-C3-C4	3.12	116.29	110.89
4	B	3	MAN	O5-C5-C6	2.84	111.66	107.20
4	B	2	NAG	C4-C3-C2	2.29	114.38	111.02
4	B	3	MAN	O5-C5-C4	-2.15	105.59	110.83
4	B	4	MAN	C3-C4-C5	2.06	113.92	110.24
4	B	4	MAN	O5-C5-C6	2.02	110.37	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4	MAN	O5-C5-C6-O6
4	B	4	MAN	C4-C5-C6-O6
4	B	3	MAN	C4-C5-C6-O6
4	B	5	MAN	O5-C5-C6-O6
4	B	3	MAN	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4	MAN	1	0

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z  > 2$
6	PO4	A	603	5	4,4,4	0.89	0	6,6,6	0.38	0
6	PO4	A	609	-	4,4,4	1.22	0	6,6,6	0.42	0
6	PO4	A	610	-	4,4,4	0.60	0	6,6,6	0.43	0
8	EDO	A	612	-	3,3,3	0.31	0	2,2,2	0.48	0
7	PG4	A	611	-	12,12,12	0.34	0	11,11,11	0.27	0

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
8	EDO	A	612	-	-	1/1/1/1	-
7	PG4	A	611	-	-	7/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	611	PG4	O3-C5-C6-O4
7	A	611	PG4	O1-C1-C2-O2
7	A	611	PG4	O4-C7-C8-O5
8	A	612	EDO	O1-C1-C2-O2
7	A	611	PG4	C3-C4-O3-C5
7	A	611	PG4	C1-C2-O2-C3
7	A	611	PG4	C8-C7-O4-C6
7	A	611	PG4	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	612	EDO	4	0
7	A	611	PG4	5	0

## 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	H	118/233 (50%)	1.50	38 (32%)	0 0	57, 94, 132, 148	0
2	L	108/215 (50%)	1.35	27 (25%)	0 0	51, 90, 126, 141	0
3	A	523/529 (98%)	-0.02	18 (3%)	45 47	33, 53, 77, 114	0
All	All	749/977 (76%)	0.42	83 (11%)	5 5	33, 59, 116, 148	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	12	SER	9.4
2	L	13	LEU	7.4
1	H	11	LEU	7.3
2	L	84	PHE	7.0
2	L	104	TYR	6.6
1	H	116	THR	6.1
1	H	112	GLY	5.7
3	A	378	GLU	4.9
2	L	17	GLU	4.9
2	L	10	THR	4.9
2	L	107	ILE	4.8
1	H	106	LEU	4.8
1	H	15	SER	4.8
1	H	27	GLY	4.7
1	H	119	SER	4.6
1	H	74	SER	4.5
1	H	83	SER	4.4
2	L	11	LEU	4.4
1	H	64	LYS	4.3
1	H	9	PRO	4.3
1	H	43	LYS	4.2
1	H	114	LEU	4.2
1	H	41	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	118	SER	3.9
2	L	24	ARG	3.8
1	H	111	GLN	3.8
2	L	18	ARG	3.7
2	L	14	SER	3.5
1	H	92	ILE	3.5
3	A	379	MET	3.5
2	L	79	LEU	3.5
1	H	115	VAL	3.4
2	L	42	GLY	3.4
1	H	30	ARG	3.4
3	A	377	ASP	3.3
2	L	37	TYR	3.3
1	H	109	TRP	3.2
2	L	108	LYS	3.2
3	A	380	PHE	3.1
1	H	117	VAL	3.0
2	L	41	PRO	2.9
2	L	47	LEU	2.9
1	H	45	LEU	2.9
1	H	84	SER	2.9
2	L	8	PRO	2.9
2	L	85	GLY	2.8
1	H	29	ILE	2.8
1	H	8	GLY	2.7
3	A	112	ALA	2.7
1	H	86	THR	2.7
2	L	99	PHE	2.7
2	L	76	ILE	2.6
2	L	69	GLY	2.6
1	H	105	SER	2.5
1	H	73	THR	2.5
3	A	140	LEU	2.5
3	A	218	LEU	2.4
3	A	402	ASN	2.4
3	A	363	LEU	2.4
1	H	37	ILE	2.4
3	A	56	ARG	2.4
3	A	81	LEU	2.4
1	H	96	ALA	2.4
1	H	5	GLN	2.3
1	H	17	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	114	ALA	2.3
1	H	24	VAL	2.3
1	H	100	TYR	2.3
3	A	113	MET	2.3
1	H	65	SER	2.2
2	L	102	GLY	2.2
1	H	66	ARG	2.2
2	L	72	PHE	2.2
1	H	28	SER	2.1
2	L	77	SER	2.1
2	L	105	LEU	2.1
3	A	84	GLY	2.1
2	L	88	TYR	2.1
3	A	83	ALA	2.1
3	A	333	ASN	2.1
3	A	173	ILE	2.0
1	H	110	GLY	2.0
3	A	115	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](#)

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(Å <sup>2</sup> )	Q<0.9
4	MAN	B	4	11/12	0.24	0.37	112,118,125,128	0
4	MAN	B	3	11/12	0.64	0.30	118,132,135,145	0
4	MAN	B	5	11/12	0.70	0.33	108,120,131,133	0
4	NAG	B	2	14/15	0.91	0.26	84,95,101,110	0
4	NAG	B	1	14/15	0.92	0.12	54,59,67,75	0

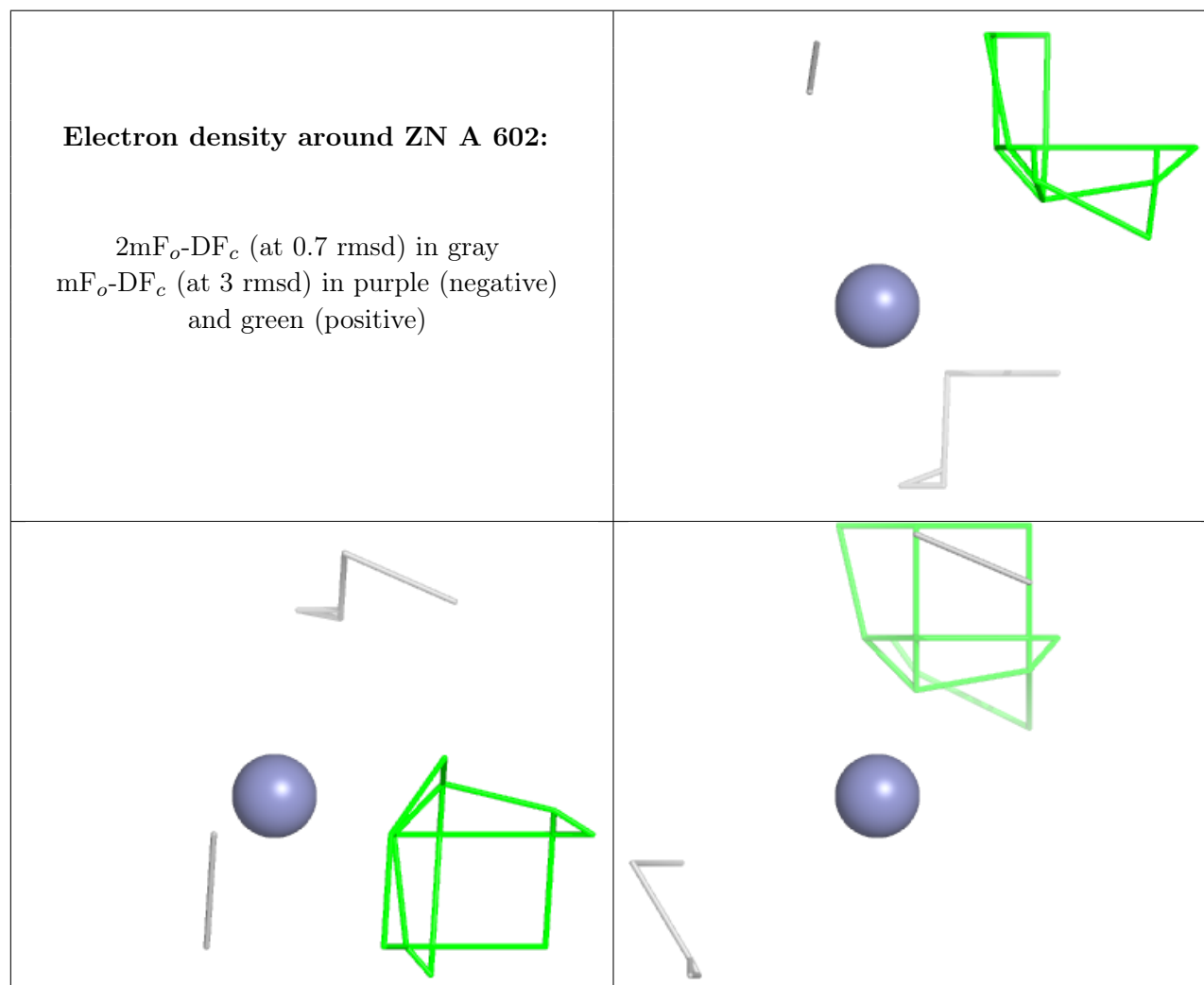
## 6.4 Ligands [i](#)

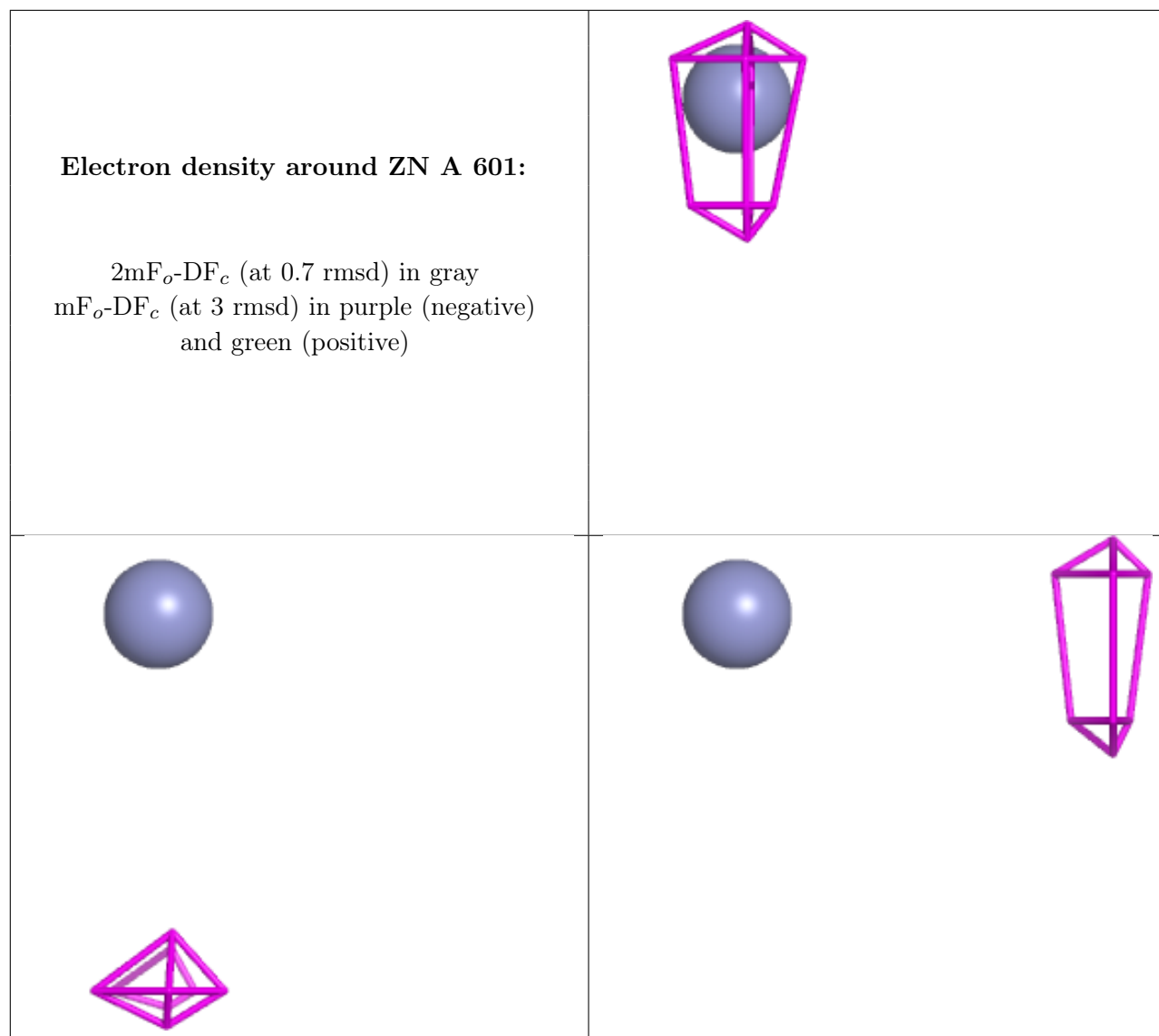
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(Å <sup>2</sup> )	Q<0.9
7	PG4	A	611	13/13	0.84	0.16	44,61,75,76	0
6	PO4	A	610	5/5	0.86	0.17	92,93,102,104	0
8	EDO	A	612	4/4	0.88	0.43	53,59,64,65	0
6	PO4	A	603	5/5	0.98	0.09	51,52,64,68	0
5	ZN	A	602	1/1	0.98	0.10	59,59,59,59	0
6	PO4	A	609	5/5	0.98	0.08	54,54,57,59	0
5	ZN	A	601	1/1	0.99	0.12	44,44,44,44	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.