

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 04:16 pm BST

PDB ID	:	8CC3
Title	:	Vibrio cholerae GbpA (LPMO domain)
Authors	:	Montserrat-Canals, M.; Sorensen, H.V.; Cordara, G.; Krengel, U.
Deposited on		
Resolution	:	1.13 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

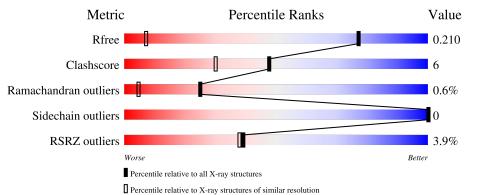
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.13 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1168 (1.14-1.10)
Clashscore	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	180	3% 92%	8%			
1	В	180	87%	12% •			



2 Entry composition (i)

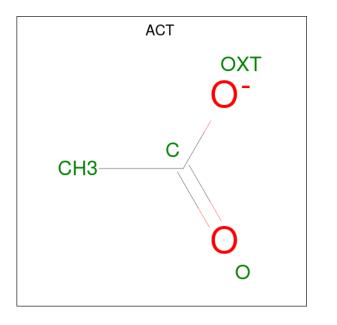
There are 6 unique types of molecules in this entry. The entry contains 3526 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GlcNAc-binding protein A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	180	Total	С	Ν	Ο	\mathbf{S}	0	30	0
		160	1655	1041	288	318	8	0		
1	В	180	Total	С	Ν	Ο	S	0	28	0
	D	180	1601	1000	279	314	8	0	28	

• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



N	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
	2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Cu 1 1	0	0
3	В	1	Total Cu 1 1	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	4	Total Zn 4 4	0	0
4	В	3	Total Zn 3 3	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Na 1 1	0	0

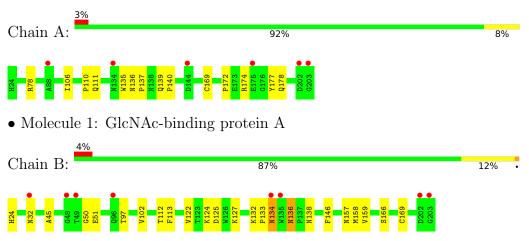
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	124	Total O 124 124	0	0
6	В	128	Total O 128 128	0	0



3 Residue-property plots (i)

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: GlcNAc-binding protein A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	74.91Å 89.10Å 47.13Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.13 - 1.13	Depositor
Resolution (A)	47.14 - 1.13	EDS
% Data completeness	98.6 (47.13-1.13)	Depositor
(in resolution range)	$98.6\ (47.14-1.13)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.89 (at 1.13 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
B B.	0.173 , 0.201	Depositor
R, R_{free}	0.182 , 0.210	DCC
R_{free} test set	5893 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	9.7	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 36.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3526	wwPDB-VP
Average B, all atoms $(Å^2)$	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: ZN, CU, ACT, NA

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/1699	0.79	2/2313~(0.1%)	
1	В	0.45	0/1655	0.79	0/2260	
All	All	0.45	0/3354	0.79	2/4573~(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
1	А	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	177[A]	TYR	CB-CG-CD1	5.16	124.09	121.00
1	А	177[B]	TYR	CB-CG-CD1	5.16	124.09	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain		• -	Group
1	А	78[A]	ARG	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1655	0	1552	10	0
1	В	1601	0	1471	29	0
2	А	8	0	6	1	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	4	0	0	0	0
4	В	3	0	0	0	0
5	В	1	0	0	0	0
6	А	124	0	0	0	0
6	В	128	0	0	1	0
All	All	3526	0	3029	39	0

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.

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 6.

All (39) 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:B:125[B]:ASP:OD2	1:B:127:LYS:HE3	1.73	0.89
1:B:158[A]:MET:O	1:B:158[A]:MET:HG2	1.75	0.86
1:B:113:PHE:HE2	1:B:169[B]:CYS:SG	2.02	0.82
1:B:113:PHE:CE2	1:B:169[B]:CYS:SG	2.78	0.75
1:B:132[B]:LYS:CB	1:B:132[B]:LYS:NZ	2.57	0.67
1:B:132[B]:LYS:NZ	1:B:132[B]:LYS:HB2	2.09	0.67
2:A:301:ACT:H2	1:B:24:HIS:CD2	2.34	0.63
1:B:32[B]:ASN:ND2	1:B:32[B]:ASN:H	2.01	0.57
1:B:136[B]:ASN:HD22	1:B:136[B]:ASN:C	2.08	0.57
1:B:124:LYS:NZ	1:B:125[A]:ASP:OD2	2.34	0.56
1:B:97:THR:HA	1:B:138[A]:ASN:HA	1.88	0.56
1:B:157[A]:ASN:O	1:B:159:VAL:HG13	2.07	0.55
1:B:133[B]:PRO:O	1:B:134[B]:ASN:HB2	2.06	0.55
1:B:132[B]:LYS:HB2	1:B:132[B]:LYS:HZ2	1.70	0.54
1:B:136[B]:ASN:HD22	1:B:138[B]:ASN:H	1.57	0.53
1:B:122:VAL:HG13	1:B:158[A]:MET:O	2.08	0.53
1:A:139[A]:GLN:HG3	1:A:140:PRO:HD2	1.92	0.51
1:B:132[B]:LYS:CB	1:B:132[B]:LYS:HZ3	2.26	0.49
1:A:172:PRO:HB2	1:A:174[B]:ARG:NH1	2.28	0.48
1:B:32[B]:ASN:CG	1:B:166[B]:SER:OG	2.51	0.48
1:B:51[B]:GLU:HB3	1:B:102:VAL:CG2	2.44	0.48

Continued on next page...



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:136:ASN:ND2	1:A:139[B]:GLN:HG2	2.29	0.47
1:B:45[A]:ALA:HB1	1:B:50[A]:GLY:HA2	1.97	0.46
1:A:106:ILE:HG13	1:A:111[B]:GLN:HE21	1.81	0.46
1:B:51[B]:GLU:HB3	1:B:102:VAL:HG21	1.98	0.46
1:A:110:PRO:HA	1:A:169[B]:CYS:O	2.16	0.46
1:B:132[B]:LYS:HG3	1:B:146:PHE:C	2.36	0.46
1:B:158[A]:MET:HB3	6:B:489:HOH:O	2.16	0.45
1:B:51[B]:GLU:OE1	1:B:102:VAL:HG22	2.16	0.45
1:A:139[A]:GLN:CG	1:A:140:PRO:HD2	2.47	0.44
1:B:32[B]:ASN:H	1:B:32[B]:ASN:HD22	1.63	0.44
1:A:139[A]:GLN:CD	1:A:140:PRO:HD2	2.38	0.43
1:B:132[B]:LYS:HZ3	1:B:132[B]:LYS:HB3	1.85	0.42
1:B:32[B]:ASN:OD1	1:B:112:THR:HG22	2.21	0.41
1:B:125[B]:ASP:OD1	1:B:125[B]:ASP:C	2.59	0.41
1:A:174[A]:ARG:CB	1:A:178[A]:GLN:HG3	2.51	0.41
1:A:135:TRP:CZ3	1:A:137:PRO:HA	2.56	0.41
1:B:32[B]:ASN:HB2	1:B:112:THR:HG21	2.03	0.41
1:A:139[B]:GLN:NE2	1:A:139[B]:GLN:HA	2.36	0.40

Continued from previous page...

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	А	209/180~(116%)	204 (98%)	5(2%)	0	100	100
1	В	206/180~(114%)	197~(96%)	5(2%)	4(2%)	8	0
All	All	415/360~(115%)	401 (97%)	10 (2%)	4 (1%)	25	1

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	134[A]	ASN
1	В	134[B]	ASN
1	В	136[A]	ASN
1	В	136[B]	ASN

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	А	175/147~(119%)	175 (100%)	0	100 100		
1	В	171/147~(116%)	171 (100%)	0	100 100		
All	All	346/294~(118%)	346 (100%)	0	100 100		

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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).

Mal	Mal Type Chain B		Image: Algorithm of the second seco		ond leng	gths	В	Bond ang	gles	
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	ACT	А	301	4	3,3,3	0.86	0	3,3,3	0.52	0
2	ACT	А	302	4	3,3,3	0.88	0	3,3,3	1.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ACT	1	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 (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^{th} 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	А	180/180~(100%)	0.39	6 (3%) 46 45	8, 11, 21, 38	0
1	В	180/180~(100%)	0.55	8 (4%) 34 32	7, 12, 20, 40	0
All	All	360/360~(100%)	0.47	14 (3%) 39 38	7, 12, 20, 40	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	В	203	GLY	8.3	
1	В	202	ASP	6.7	
1	А	203	GLY	5.5	
1	А	202	ASP	4.8	
1	А	175[A]	GLU	3.2	
1	В	49[A]	THR	3.1	
1	В	32[A]	ASN	2.8	
1	В	48[A]	GLY	2.5	
1	А	134	ASN	2.4	
1	В	96	GLN	2.3	
1	А	144[A]	ASP	2.3	
1	В	134[A]	ASN	2.2	
1	А	88[A]	ALA	2.1	
1	В	135[A]	TRP	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.



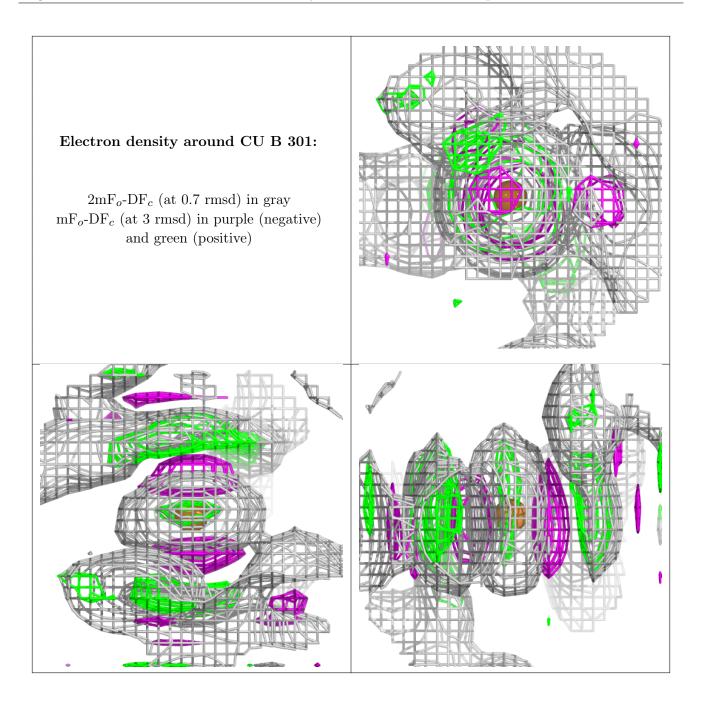
6.4 Ligands (i)

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^{th} 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.

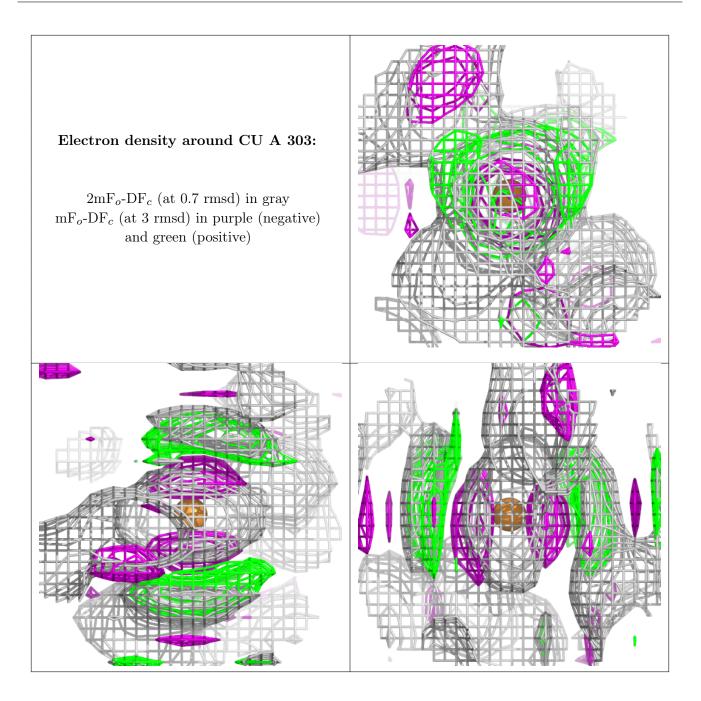
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
2	ACT	А	301	4/4	0.90	0.15	$15,\!16,\!17,\!24$	0
2	ACT	А	302	4/4	0.93	0.12	14, 16, 18, 22	0
3	CU	В	301	1/1	0.99	0.07	$9,\!9,\!9,\!9$	0
4	ZN	А	304	1/1	0.99	0.06	10,10,10,10	0
4	ZN	А	305	1/1	0.99	0.02	20,20,20,20	1
4	ZN	А	307	1/1	0.99	0.06	$12,\!12,\!12,\!12$	1
4	ZN	В	302	1/1	0.99	0.05	8,8,8,8	1
4	ZN	В	303	1/1	0.99	0.03	$12,\!12,\!12,\!12$	0
4	ZN	В	304	1/1	0.99	0.07	$17,\!17,\!17,\!17$	1
5	NA	В	305	1/1	0.99	0.13	$9,\!9,\!9,\!9$	1
4	ZN	А	306	1/1	1.00	0.04	8,8,8,8	1
3	CU	A	303	1/1	1.00	0.04	8,8,8,8	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.

