



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2025 – 10:14 AM JST

PDB ID : 8ZXG / pdb\_00008zxg  
Title : Crystal structure of Paraoxonase from Bacillus sp. strain S3wahi  
Authors : Azman, A.A.; Muhd Noor, N.D.; Leow, A.T.C.; Mohd Noor, S.A.; Mohamad Ali, M.S.  
Deposited on : 2024-06-14  
Resolution : 1.49 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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 Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

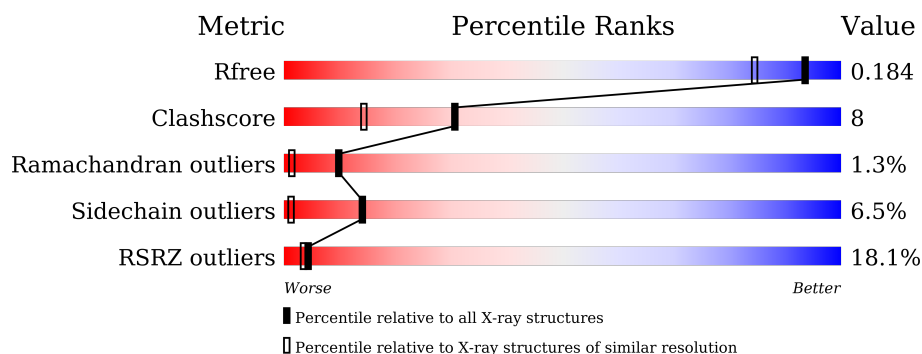
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.49 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))
$R_{free}$	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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	A	316	<div> <div>18%</div> <div>80%</div> <div>12%</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	GOL	A	401	-	-	X	-
3	MG	A	449	-	-	-	X

## 2 Entry composition [i](#)

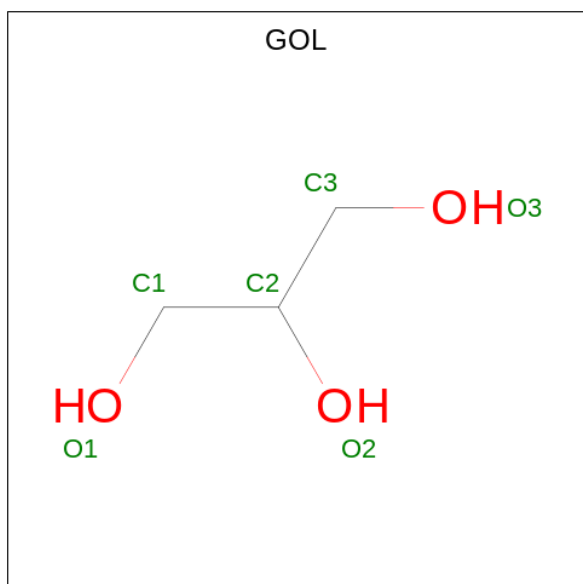
There are 5 unique types of molecules in this entry. The entry contains 2622 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Paraoxonase from *Bacillus* sp. strain S3wahi.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2429	1564	408	446	11	0	11	0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	Mg	0	0
			58	58		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

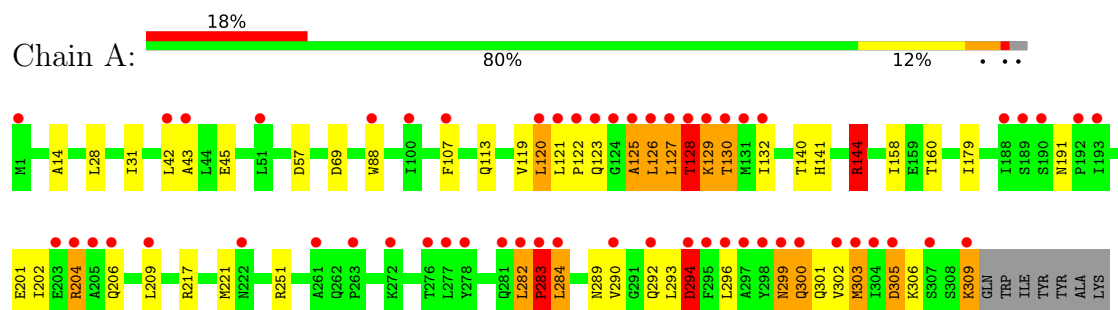
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		

### 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: Paraoxonase from *Bacillus* sp. strain S3wahi



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.82Å 77.82Å 135.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 1.49 39.01 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.01-1.49) 99.9 (39.01-1.49)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.183 , 0.195 0.185 , 0.184	Depositor DCC
$R_{free}$ test set	3501 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.1	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	2622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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, MG, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.81	2/2515 (0.1%)	1.20	10/3422 (0.3%)

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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	PRO	C-O	8.11	1.34	1.24
1	A	127	LEU	C-N	6.16	1.42	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	PRO	N-CA-CB	-11.54	91.14	103.25
1	A	202	ILE	N-CA-C	-8.01	103.09	111.58
1	A	294	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	128	THR	CA-CB-OG1	6.25	118.97	109.60
1	A	283	PRO	O-C-N	6.10	130.88	122.64
1	A	107	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	128	THR	OG1-CB-CG2	-5.59	98.12	109.30
1	A	127	LEU	CD1-CG-CD2	-5.50	98.69	110.80
1	A	209	LEU	N-CA-CB	5.46	118.14	110.12
1	A	300	GLN	N-CA-CB	5.17	118.67	110.55

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ALA	Peptide
1	A	144[A]	ARG	Sidechain
1	A	144[B]	ARG	Sidechain
1	A	204	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	A	2429	0	2412	40	41
2	A	54	0	70	5	0
3	A	58	0	0	0	0
4	A	2	0	0	0	0
5	A	79	0	0	3	3
All	All	2622	0	2482	41	42

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 (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144[A]:ARG:HH11	1:A:144[A]:ARG:HG2	0.92	1.08
1:A:144[A]:ARG:HG2	1:A:144[A]:ARG:NH1	1.68	1.01
1:A:144[A]:ARG:HH11	1:A:144[A]:ARG:CG	1.85	0.80
1:A:122:PRO:HA	1:A:126:LEU:HD23	1.64	0.80
1:A:119:VAL:HG23	1:A:120:LEU:HD13	1.70	0.74
1:A:57:ASP:OD2	2:A:401:GOL:H32	1.90	0.71
1:A:144[A]:ARG:NH1	1:A:144[A]:ARG:CG	2.49	0.64
1:A:57:ASP:CG	2:A:401:GOL:H32	2.26	0.61
1:A:206:GLN:HE21	1:A:290:VAL:HG12	1.65	0.61
1:A:126:LEU:C	1:A:128:THR:H	2.12	0.58
1:A:251:ARG:HH11	1:A:284:LEU:HD12	1.68	0.57
1:A:201:GLU:OE2	1:A:204:ARG:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:C	1:A:296:LEU:H	2.13	0.56
1:A:294:ASP:O	1:A:296:LEU:N	2.40	0.55
1:A:293:LEU:C	1:A:294:ASP:O	2.46	0.54
1:A:206:GLN:NE2	1:A:290:VAL:HG12	2.24	0.52
1:A:126:LEU:C	1:A:128:THR:N	2.68	0.51
1:A:302:VAL:O	1:A:303:MET:CB	2.59	0.51
1:A:301:GLN:CB	5:A:561:HOH:O	2.60	0.50
1:A:57:ASP:OD1	2:A:401:GOL:H32	2.11	0.50
1:A:289:ASN:HB3	1:A:309[B]:LYS:HE2	1.93	0.49
1:A:299:ASN:N	1:A:299:ASN:OD1	2.46	0.48
1:A:31:ILE:HD13	1:A:179:ILE:HD13	1.97	0.47
1:A:130:THR:C	1:A:132:ILE:H	2.23	0.47
1:A:125:ALA:HB2	1:A:129:LYS:HD3	1.97	0.46
1:A:251:ARG:NH1	1:A:284:LEU:HD12	2.30	0.46
2:A:401:GOL:H12	5:A:502:HOH:O	2.16	0.46
1:A:121:LEU:O	1:A:122:PRO:C	2.59	0.45
1:A:126:LEU:HA	1:A:126:LEU:HD13	1.53	0.45
1:A:126:LEU:HB2	1:A:128:THR:O	2.17	0.44
1:A:158[C]:ILE:HG12	1:A:160:THR:HG23	1.98	0.44
1:A:14:ALA:HB3	2:A:403:GOL:H32	1.99	0.44
1:A:282:LEU:HD12	1:A:282:LEU:O	2.18	0.43
1:A:292:GLN:O	1:A:294:ASP:O	2.36	0.43
1:A:140:THR:OG1	1:A:141:HIS:HD2	2.01	0.43
1:A:191:ASN:HD22	1:A:284:LEU:HD11	1.85	0.42
1:A:158[C]:ILE:HG13	1:A:217:ARG:NH1	2.36	0.41
1:A:129:LYS:O	1:A:130:THR:HG23	2.19	0.41
1:A:69:ASP:OD1	5:A:501:HOH:O	2.21	0.41
1:A:113:GLN:HA	1:A:305:ASP:O	2.21	0.41
1:A:217:ARG:O	1:A:221[A]:MET:HG3	2.21	0.41

All (42) 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)
1:A:42:LEU:C	1:A:127:LEU:CA[7_555]	0.66	1.54
1:A:43:ALA:CA	1:A:127:LEU:CG[7_555]	0.74	1.46
1:A:42:LEU:O	1:A:127:LEU:N[7_555]	0.75	1.45
1:A:42:LEU:CB	1:A:128:THR:N[7_555]	0.94	1.26
1:A:42:LEU:CB	1:A:127:LEU:C[7_555]	1.06	1.14
1:A:43:ALA:N	1:A:127:LEU:CA[7_555]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:CG	1:A:128:THR:CA[7_555]	1.11	1.09
1:A:43:ALA:CB	1:A:127:LEU:CG[7_555]	1.17	1.03
1:A:43:ALA:N	1:A:127:LEU:CB[7_555]	1.28	0.92
1:A:43:ALA:O	1:A:127:LEU:CD1[7_555]	1.29	0.91
1:A:43:ALA:CA	1:A:127:LEU:CB[7_555]	1.29	0.91
1:A:42:LEU:CA	1:A:127:LEU:C[7_555]	1.31	0.89
1:A:42:LEU:CD1	1:A:128:THR:CB[7_555]	1.40	0.80
1:A:42:LEU:C	1:A:127:LEU:N[7_555]	1.43	0.77
1:A:42:LEU:CD1	1:A:128:THR:CA[7_555]	1.46	0.74
1:A:43:ALA:CB	1:A:127:LEU:CD2[7_555]	1.50	0.70
1:A:42:LEU:O	1:A:127:LEU:CA[7_555]	1.54	0.66
1:A:42:LEU:CB	1:A:127:LEU:O[7_555]	1.58	0.62
1:A:42:LEU:CB	1:A:128:THR:CA[7_555]	1.63	0.57
1:A:43:ALA:C	1:A:127:LEU:CD1[7_555]	1.63	0.57
1:A:126:LEU:O	5:A:567:HOH:O[7_555]	1.66	0.54
1:A:42:LEU:C	1:A:127:LEU:C[7_555]	1.71	0.49
1:A:42:LEU:CD1	1:A:128:THR:OG1[7_555]	1.74	0.46
5:A:522:HOH:O	5:A:579:HOH:O[4_444]	1.76	0.44
1:A:43:ALA:CA	1:A:127:LEU:CD1[7_555]	1.80	0.40
1:A:43:ALA:C	1:A:127:LEU:CG[7_555]	1.82	0.38
1:A:42:LEU:CA	1:A:128:THR:N[7_555]	1.84	0.36
1:A:42:LEU:CG	1:A:128:THR:N[7_555]	1.89	0.31
1:A:42:LEU:CA	1:A:127:LEU:CA[7_555]	1.90	0.30
1:A:42:LEU:CA	1:A:127:LEU:O[7_555]	1.92	0.28
1:A:45:GLU:OE2	1:A:125:ALA:CB[7_555]	1.95	0.25
1:A:42:LEU:CD2	1:A:128:THR:CA[7_555]	1.97	0.23
1:A:42:LEU:N	1:A:127:LEU:O[7_555]	1.99	0.21
1:A:43:ALA:CB	1:A:127:LEU:CB[7_555]	2.00	0.20
1:A:42:LEU:O	1:A:126:LEU:C[7_555]	2.04	0.16
1:A:42:LEU:CD2	1:A:128:THR:C[7_555]	2.06	0.14
1:A:43:ALA:CA	1:A:127:LEU:CA[7_555]	2.12	0.08
1:A:42:LEU:CD2	1:A:129:LYS:N[7_555]	2.13	0.07
1:A:43:ALA:N	1:A:127:LEU:CG[7_555]	2.13	0.07
1:A:42:LEU:C	1:A:127:LEU:CB[7_555]	2.15	0.05
1:A:42:LEU:CG	1:A:128:THR:CB[7_555]	2.19	0.01
1:A:127:LEU:CD2	5:A:562:HOH:O[7_555]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/316 (101%)	298 (94%)	16 (5%)	4 (1%)	10	1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	PRO
1	A	303	MET
1	A	305	ASP
1	A	294	ASP

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/280 (92%)	239 (93%)	19 (7%)	11	1

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	88[A]	TRP
1	A	88[B]	TRP
1	A	120	LEU
1	A	123	GLN
1	A	126	LEU
1	A	128	THR

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Mol	Chain	Res	Type
1	A	129	LYS
1	A	130	THR
1	A	144[A]	ARG
1	A	144[B]	ARG
1	A	282	LEU
1	A	283	PRO
1	A	284	LEU
1	A	299	ASN
1	A	300	GLN
1	A	306	LYS
1	A	309[A]	LYS
1	A	309[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	141	HIS
1	A	191	ASN
1	A	222	ASN
1	A	257	ASN
1	A	292	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 60 are monoatomic - leaving 9 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	$\# Z  > 2$
2	GOL	A	402[A]	-	5,5,5	0.15	0	5,5,5	0.37	0
2	GOL	A	405[B]	-	5,5,5	0.28	0	5,5,5	0.53	0
2	GOL	A	405[A]	-	5,5,5	0.17	0	5,5,5	0.42	0
2	GOL	A	403	-	5,5,5	0.46	0	5,5,5	1.00	0
2	GOL	A	406	-	5,5,5	0.16	0	5,5,5	0.39	0
2	GOL	A	407	-	5,5,5	0.18	0	5,5,5	0.31	0
2	GOL	A	402[B]	-	5,5,5	0.24	0	5,5,5	0.40	0
2	GOL	A	404	-	5,5,5	0.34	0	5,5,5	0.33	0
2	GOL	A	401	-	5,5,5	0.88	0	5,5,5	0.31	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
2	GOL	A	402[A]	-	-	2/4/4/4	-
2	GOL	A	405[B]	-	-	2/4/4/4	-
2	GOL	A	405[A]	-	-	3/4/4/4	-
2	GOL	A	403	-	-	4/4/4/4	-
2	GOL	A	406	-	-	2/4/4/4	-
2	GOL	A	407	-	-	2/4/4/4	-
2	GOL	A	402[B]	-	-	2/4/4/4	-
2	GOL	A	404	-	-	4/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	A	403	GOL	O1-C1-C2-C3
2	A	403	GOL	C1-C2-C3-O3
2	A	404	GOL	O1-C1-C2-C3
2	A	404	GOL	C1-C2-C3-O3
2	A	404	GOL	O2-C2-C3-O3
2	A	405[A]	GOL	O1-C1-C2-O2
2	A	405[A]	GOL	O1-C1-C2-C3
2	A	405[B]	GOL	O1-C1-C2-O2
2	A	405[B]	GOL	O1-C1-C2-C3
2	A	406	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	A	404	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-O2
2	A	406	GOL	O2-C2-C3-O3
2	A	402[B]	GOL	O1-C1-C2-O2
2	A	405[A]	GOL	O2-C2-C3-O3
2	A	402[A]	GOL	O1-C1-C2-O2
2	A	403	GOL	O2-C2-C3-O3
2	A	407	GOL	O1-C1-C2-O2
2	A	407	GOL	O1-C1-C2-C3
2	A	402[B]	GOL	O1-C1-C2-C3
2	A	402[A]	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	GOL	1	0
2	A	401	GOL	4	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	A	309/316 (97%)	1.04	56 (18%) 4 3	12, 33, 71, 144	11 (3%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	LEU	15.8
1	A	128	THR	14.4
1	A	125	ALA	9.8
1	A	284	LEU	9.5
1	A	130	THR	8.8
1	A	282	LEU	8.2
1	A	127	LEU	7.9
1	A	283	PRO	7.7
1	A	42	LEU	6.6
1	A	295	PHE	6.5
1	A	205	ALA	6.4
1	A	129	LYS	6.4
1	A	124	GLY	5.7
1	A	296	LEU	5.1
1	A	123	GLN	4.6
1	A	188	ILE	4.5
1	A	122	PRO	4.4
1	A	304	ILE	4.4
1	A	302	VAL	4.1
1	A	290	VAL	4.0
1	A	121	LEU	3.7
1	A	204	ARG	3.6
1	A	276	THR	3.3
1	A	107	PHE	3.3
1	A	303	MET	3.1
1	A	300	GLN	3.0
1	A	203	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	263	PRO	3.0
1	A	277	LEU	2.9
1	A	278	TYR	2.8
1	A	1	MET	2.8
1	A	298	TYR	2.8
1	A	132	ILE	2.7
1	A	209	LEU	2.6
1	A	193	ILE	2.6
1	A	88[A]	TRP	2.6
1	A	305	ASP	2.6
1	A	131[A]	MET	2.5
1	A	261	ALA	2.5
1	A	51	LEU	2.4
1	A	292	GLN	2.4
1	A	222	ASN	2.4
1	A	100	ILE	2.3
1	A	294	ASP	2.3
1	A	299	ASN	2.3
1	A	192	PRO	2.3
1	A	307	SER	2.3
1	A	309[A]	LYS	2.3
1	A	272	LYS	2.2
1	A	206	GLN	2.1
1	A	43	ALA	2.1
1	A	281	GLN	2.1
1	A	297	ALA	2.1
1	A	120	LEU	2.1
1	A	190	SER	2.1
1	A	189	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.



## 6.4 Ligands ⓘ

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
3	MG	A	449	1/1	0.33	0.41	119,119,119,119	0
2	GOL	A	405[B]	6/6	0.56	0.20	35,42,50,50	6
2	GOL	A	405[A]	6/6	0.56	0.20	38,43,50,51	6
3	MG	A	441	1/1	0.66	0.25	101,101,101,101	0
3	MG	A	464	1/1	0.69	0.22	83,83,83,83	0
2	GOL	A	406	6/6	0.74	0.16	58,61,65,68	0
2	GOL	A	401	6/6	0.74	0.33	98,110,117,121	0
2	GOL	A	407	6/6	0.76	0.21	54,60,67,76	0
3	MG	A	465	1/1	0.77	0.20	82,82,82,82	0
2	GOL	A	404	6/6	0.79	0.20	35,48,58,58	0
3	MG	A	435	1/1	0.82	0.18	59,59,59,59	0
3	MG	A	455	1/1	0.82	0.32	84,84,84,84	0
2	GOL	A	403	6/6	0.83	0.16	41,46,51,61	0
3	MG	A	463	1/1	0.84	0.19	62,62,62,62	0
3	MG	A	461	1/1	0.85	0.20	62,62,62,62	0
3	MG	A	462	1/1	0.87	0.16	72,72,72,72	0
3	MG	A	460	1/1	0.87	0.16	55,55,55,55	0
3	MG	A	453	1/1	0.89	0.14	54,54,54,54	0
3	MG	A	444	1/1	0.90	0.14	57,57,57,57	0
3	MG	A	427	1/1	0.90	0.15	61,61,61,61	0
2	GOL	A	402[B]	6/6	0.91	0.13	20,34,40,51	6
2	GOL	A	402[A]	6/6	0.91	0.13	21,35,46,48	6
3	MG	A	446	1/1	0.92	0.18	49,49,49,49	0
3	MG	A	429	1/1	0.92	0.17	54,54,54,54	0
3	MG	A	438	1/1	0.93	0.15	52,52,52,52	0
3	MG	A	450	1/1	0.94	0.21	54,54,54,54	0
3	MG	A	413	1/1	0.94	0.18	41,41,41,41	0
3	MG	A	411	1/1	0.94	0.11	48,48,48,48	0
3	MG	A	457	1/1	0.94	0.28	70,70,70,70	0
3	MG	A	442	1/1	0.94	0.11	54,54,54,54	0
3	MG	A	418	1/1	0.95	0.32	64,64,64,64	0
3	MG	A	458	1/1	0.95	0.09	59,59,59,59	0
3	MG	A	434	1/1	0.95	0.28	44,44,44,44	0
3	MG	A	452	1/1	0.95	0.12	49,49,49,49	0
3	MG	A	408	1/1	0.95	0.29	43,43,43,43	0
3	MG	A	454	1/1	0.95	0.09	66,66,66,66	0
3	MG	A	428	1/1	0.95	0.27	47,47,47,47	0

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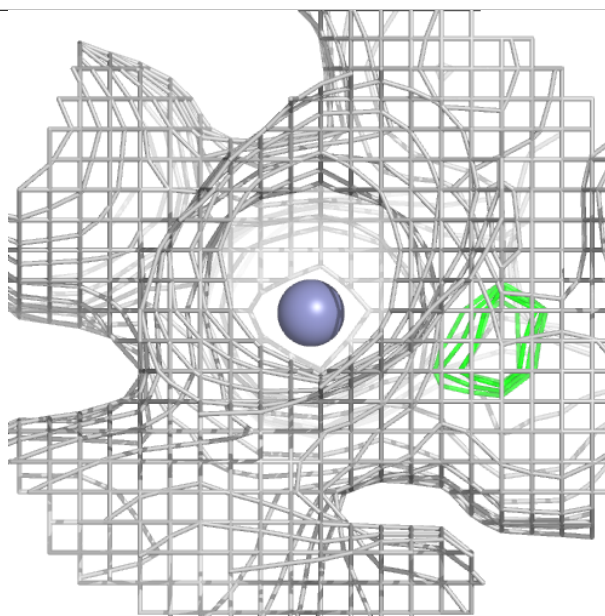
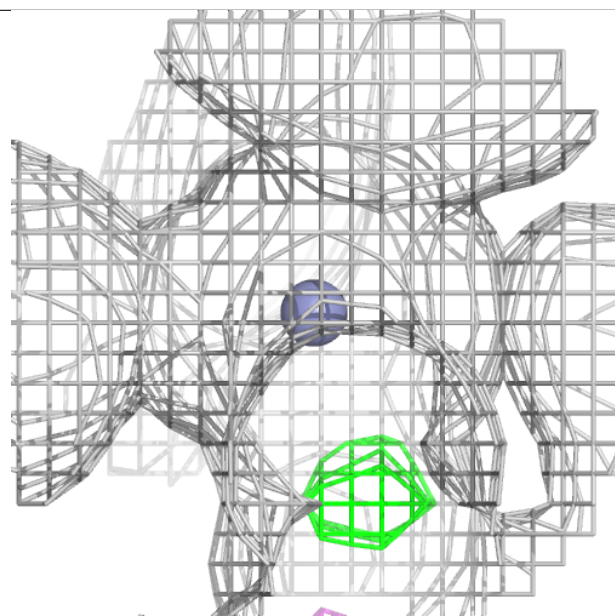
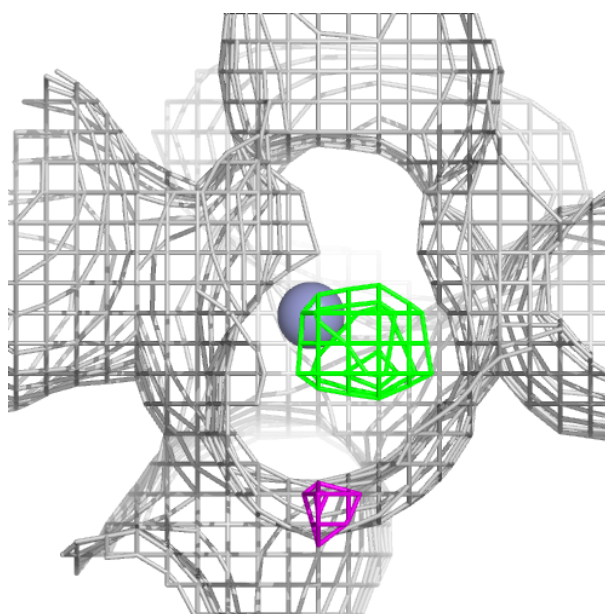
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	456	1/1	0.95	0.11	50,50,50,50	0
3	MG	A	420	1/1	0.96	0.15	48,48,48,48	0
3	MG	A	423	1/1	0.96	0.11	44,44,44,44	0
3	MG	A	440	1/1	0.96	0.09	44,44,44,44	0
3	MG	A	424	1/1	0.96	0.11	44,44,44,44	0
3	MG	A	451	1/1	0.96	0.33	55,55,55,55	0
3	MG	A	425	1/1	0.96	0.12	44,44,44,44	0
3	MG	A	443	1/1	0.97	0.13	49,49,49,49	0
3	MG	A	433	1/1	0.97	0.28	44,44,44,44	0
3	MG	A	421	1/1	0.97	0.15	40,40,40,40	0
3	MG	A	448	1/1	0.97	0.10	57,57,57,57	0
3	MG	A	459	1/1	0.97	0.08	53,53,53,53	0
3	MG	A	426	1/1	0.97	0.12	57,57,57,57	0
3	MG	A	436	1/1	0.97	0.16	44,44,44,44	0
3	MG	A	422	1/1	0.97	0.10	43,43,43,43	0
3	MG	A	410	1/1	0.97	0.27	42,42,42,42	0
3	MG	A	416	1/1	0.97	0.32	40,40,40,40	0
3	MG	A	430	1/1	0.97	0.10	34,34,34,34	0
3	MG	A	409	1/1	0.98	0.14	44,44,44,44	0
3	MG	A	445	1/1	0.98	0.11	44,44,44,44	0
3	MG	A	439	1/1	0.98	0.08	54,54,54,54	0
3	MG	A	414	1/1	0.98	0.23	48,48,48,48	0
3	MG	A	412	1/1	0.98	0.18	36,36,36,36	0
3	MG	A	431	1/1	0.98	0.07	37,37,37,37	0
3	MG	A	437	1/1	0.98	0.10	52,52,52,52	0
3	MG	A	415	1/1	0.99	0.03	29,29,29,29	0
3	MG	A	447	1/1	0.99	0.06	40,40,40,40	0
3	MG	A	419	1/1	0.99	0.04	44,44,44,44	0
3	MG	A	432	1/1	0.99	0.05	32,32,32,32	0
3	MG	A	417	1/1	0.99	0.11	42,42,42,42	0
4	ZN	A	466	1/1	1.00	0.01	24,24,24,24	0
4	ZN	A	467	1/1	1.00	0.01	23,23,23,23	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.

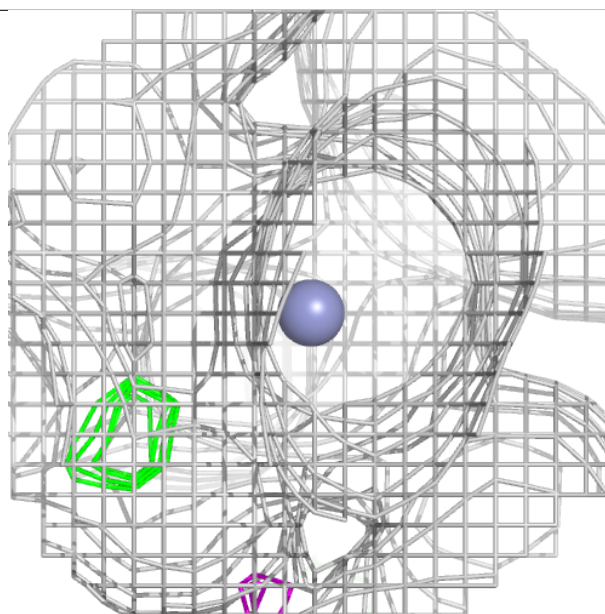
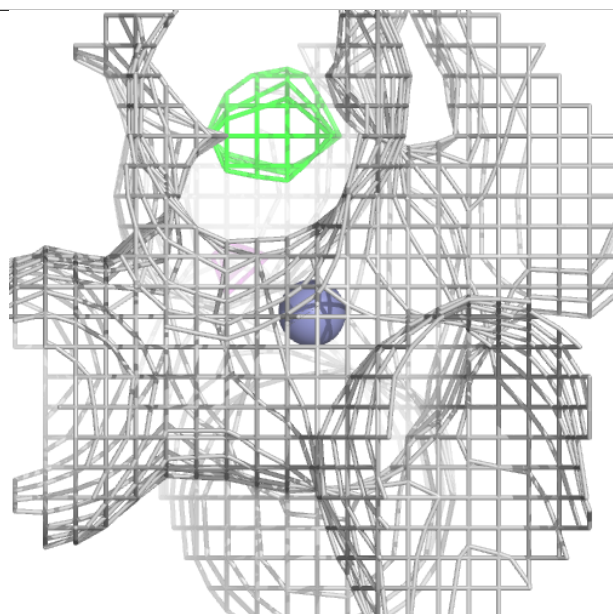
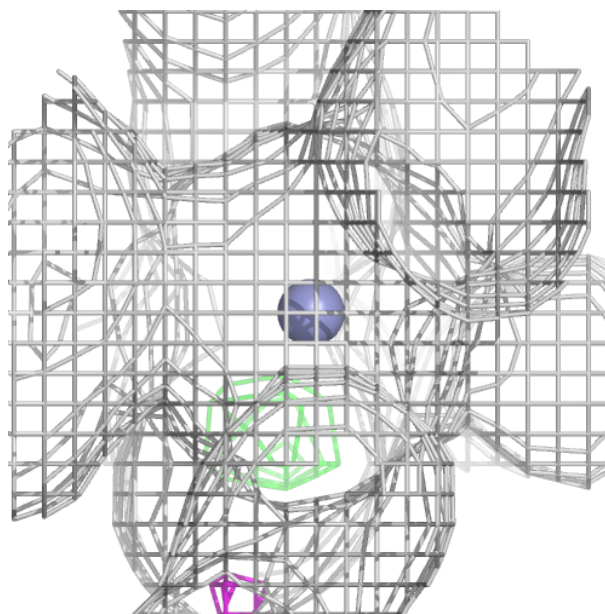
**Electron density around ZN A 466:**

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



**Electron density around ZN A 467:**

$2mF_o-DF_c$  (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.