



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2021 – 08:10 PM JST

PDB ID : 7DIF  
Title : GH127 beta-L-arabinofuranosidase HypBA1 covalently complexed with beta-L-arabinofuranose-configured cyclophellitol at 1.75-angstrom resolution  
Authors : Amaki, S.; McGregor, N.G.S.; Arakawa, T.; Yamada, C.; Borlandelli, V.; Overkleeft, H.S.; Davies, G.J.; Fushinobu, S.  
Deposited on : 2020-11-19  
Resolution : 1.75 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 : 2.16  
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) : 2.16

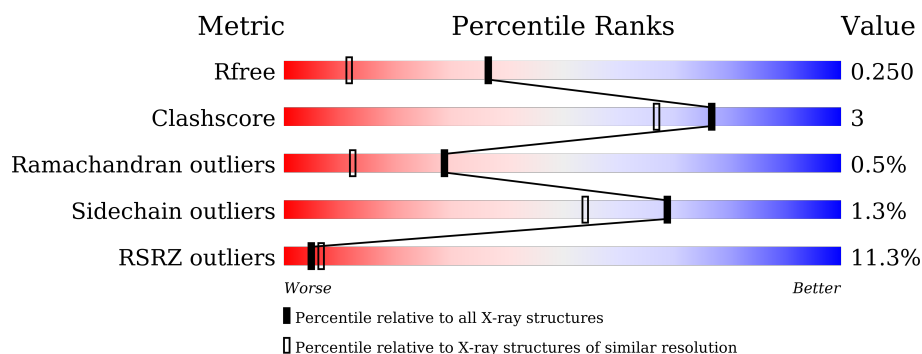
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	669	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5381 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 Non-reducing end beta-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	656	5136	3234	882	997	23	0	0	0

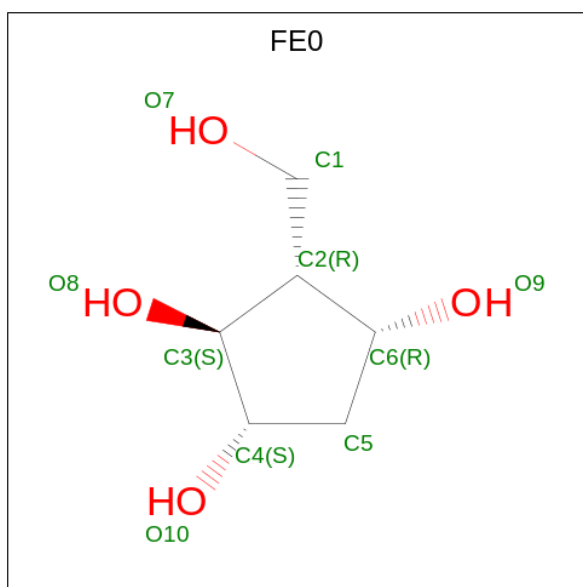
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	659	ALA	-	expression tag	UNP E8MGH8
A	660	ALA	-	expression tag	UNP E8MGH8
A	661	ALA	-	expression tag	UNP E8MGH8
A	662	LEU	-	expression tag	UNP E8MGH8
A	663	GLU	-	expression tag	UNP E8MGH8
A	664	HIS	-	expression tag	UNP E8MGH8
A	665	HIS	-	expression tag	UNP E8MGH8
A	666	HIS	-	expression tag	UNP E8MGH8
A	667	HIS	-	expression tag	UNP E8MGH8
A	668	HIS	-	expression tag	UNP E8MGH8
A	669	HIS	-	expression tag	UNP E8MGH8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (1S,2S,3R,4R)-3-(hydroxymethyl)cyclopentane-1,2,4-triol (three-letter code: FE0) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

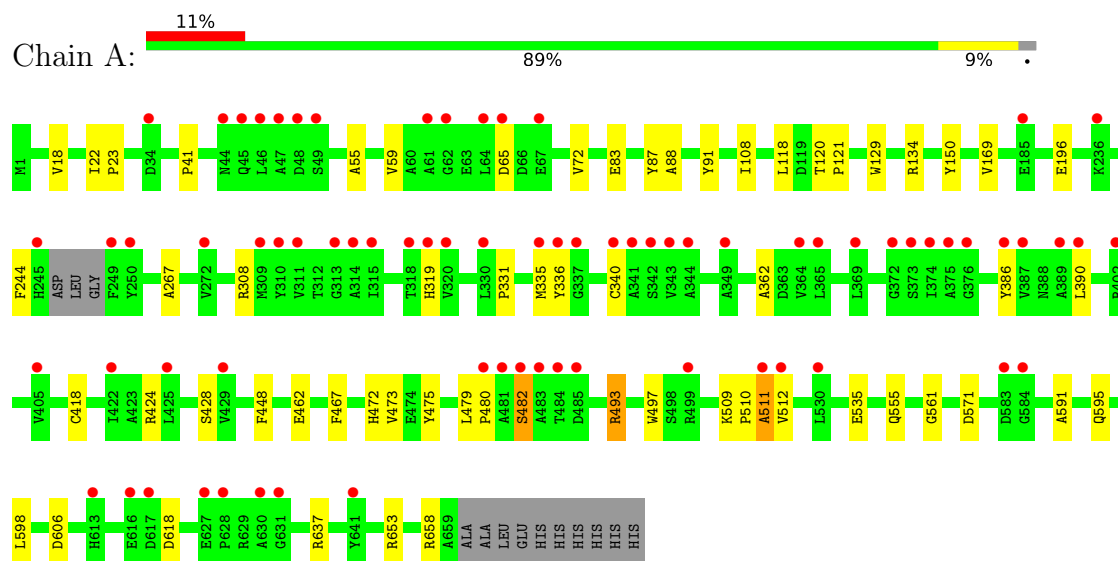
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	233	Total	O	0	0
			233	233		

### 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: Non-reducing end beta-L-arabinofuranosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.71Å 77.71Å 252.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.05 – 1.75 46.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.05-1.75) 99.9 (46.00-1.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.216 , 0.243 0.222 , 0.250	Depositor DCC
$R_{free}$ test set	4479 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: ZN, K, FE0

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	0.71	0/5257	0.87	2/7150 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	244	PHE	CB-CA-C	-5.48	99.43	110.40

There are no chirality outliers.

There are no planarity outliers.

### 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	5136	0	4900	30	0
2	A	1	0	0	0	0
3	A	10	0	0	0	0
4	A	1	0	0	0	0
5	A	233	0	0	0	0
All	All	5381	0	4900	30	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 3.

All (30) 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:362:ALA:HB3	1:A:493:ARG:HD3	1.68	0.75
1:A:510:PRO:O	1:A:511:ALA:C	2.38	0.61
1:A:335:MET:SD	1:A:390:LEU:HD13	2.41	0.61
1:A:120:THR:N	1:A:121:PRO:HD2	2.18	0.58
1:A:571:ASP:HB3	1:A:637:ARG:HG2	1.90	0.54
1:A:319:HIS:HA	1:A:336:TYR:CD1	2.45	0.51
1:A:595:GLN:HB2	1:A:598:LEU:HB3	1.93	0.51
1:A:41:PRO:HG2	1:A:386:TYR:CG	2.46	0.51
1:A:473:VAL:HG12	1:A:475:TYR:CE1	2.47	0.50
1:A:448:PHE:HB2	1:A:467:PHE:CD2	2.49	0.48
1:A:87:TYR:CD2	1:A:428:SER:HB3	2.50	0.47
1:A:83:GLU:HG2	1:A:87:TYR:CE2	2.51	0.46
1:A:18:VAL:HG12	1:A:88:ALA:HB1	1.97	0.45
1:A:72:VAL:HG23	1:A:129:TRP:CH2	2.52	0.45
1:A:510:PRO:O	1:A:512:VAL:N	2.49	0.45
1:A:472:HIS:ND1	1:A:535:GLU:OE2	2.39	0.45
1:A:55:ALA:O	1:A:59:VAL:HG23	2.17	0.44
1:A:150:TYR:CE2	1:A:169:VAL:HG12	2.53	0.44
1:A:88:ALA:HA	1:A:91:TYR:CE1	2.54	0.42
1:A:108:ILE:HG23	1:A:118:LEU:CD2	2.48	0.42
1:A:479:LEU:HD12	1:A:480:PRO:HD2	2.01	0.42
1:A:331:PRO:O	1:A:335:MET:HB3	2.20	0.41
1:A:462:GLU:O	1:A:475:TYR:HA	2.20	0.41
1:A:555:GLN:OE1	1:A:653:ARG:NH2	2.48	0.41
1:A:340:CYS:SG	1:A:418:CYS:HA	2.61	0.41
1:A:22:ILE:N	1:A:23:PRO:HD2	2.35	0.41
1:A:591:ALA:HB3	1:A:606:ASP:HB2	2.03	0.41
1:A:267:ALA:O	1:A:308:ARG:NH1	2.54	0.40
1:A:87:TYR:CG	1:A:428:SER:HB3	2.57	0.40
1:A:497:TRP:CZ3	1:A:561:GLY:HA2	2.56	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	A	652/669 (98%)	623 (96%)	26 (4%)	3 (0%)	29	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
1	A	511	ALA
1	A	482	SER

### 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	536/546 (98%)	529 (99%)	7 (1%)	69	54

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	A	134	ARG
1	A	424	ARG
1	A	482	SER
1	A	509	LYS
1	A	618	ASP
1	A	658	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	319	HIS
1	A	578	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
3	FE0	A	702	1	10,10,10	0.76	0	11,14,14	1.49	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FE0	A	702	1	-	0/2/18/18	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FE0	C5-C6-C2	3.58	109.50	104.13

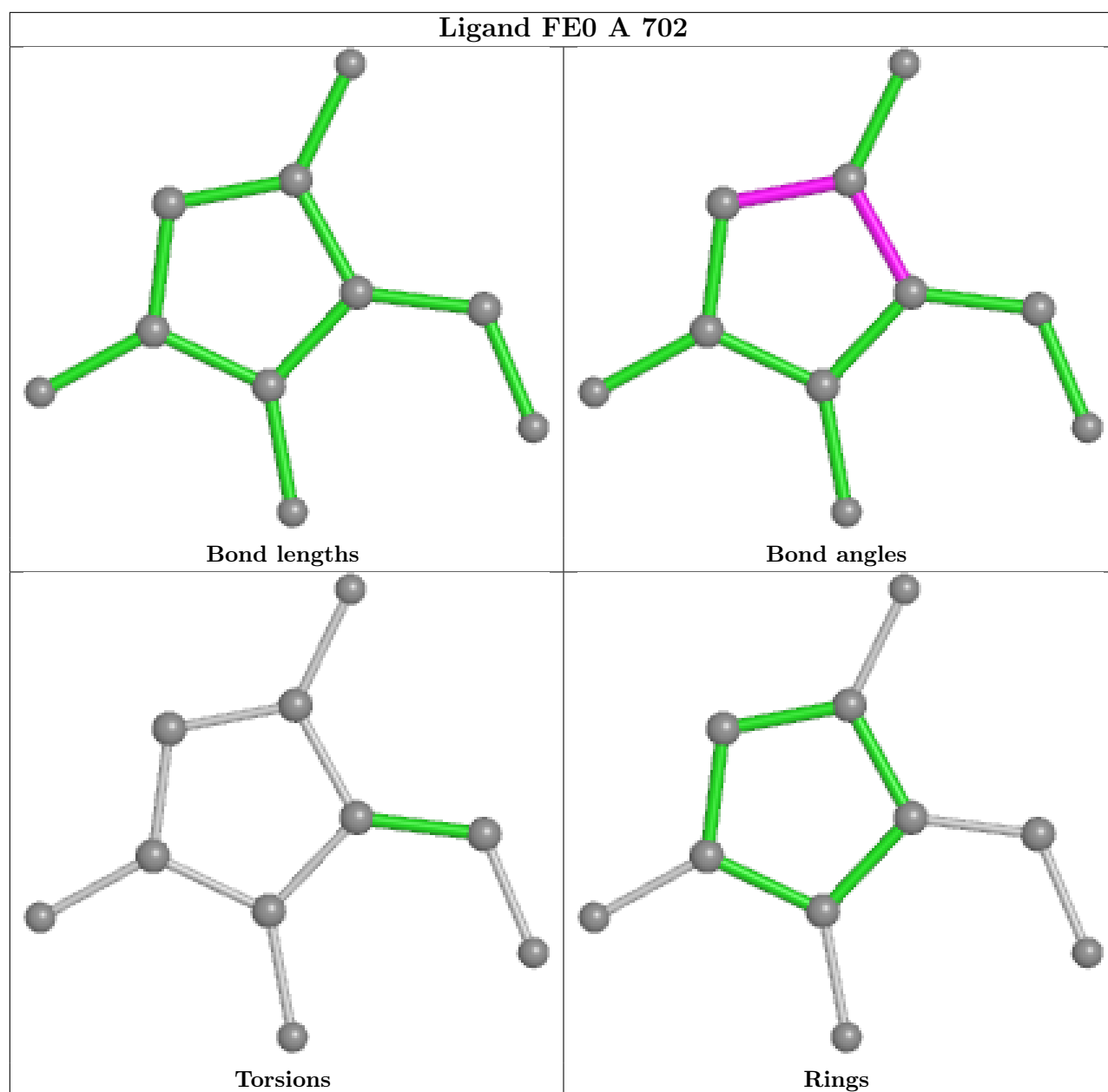
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	656/669 (98%)	0.55	74 (11%) 5 7	31, 43, 67, 127	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	LEU	9.0
1	A	483	ALA	8.5
1	A	484	THR	7.4
1	A	249	PHE	6.2
1	A	485	ASP	4.5
1	A	48	ASP	4.4
1	A	65	ASP	4.4
1	A	49	SER	4.4
1	A	315	ILE	4.1
1	A	387	VAL	4.1
1	A	64	LEU	3.9
1	A	343	VAL	3.8
1	A	374	ILE	3.8
1	A	480	PRO	3.7
1	A	584	GLY	3.7
1	A	628	PRO	3.7
1	A	482	SER	3.6
1	A	512	VAL	3.4
1	A	631	GLY	3.2
1	A	481	ALA	3.2
1	A	340	CYS	3.1
1	A	320	VAL	3.1
1	A	250	TYR	3.1
1	A	405	VAL	3.1
1	A	341	ALA	2.9
1	A	61	ALA	2.9
1	A	245	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	45	GLN	2.7
1	A	310	TYR	2.6
1	A	330	LEU	2.6
1	A	336	TYR	2.6
1	A	386	TYR	2.6
1	A	511	ALA	2.6
1	A	369	LEU	2.6
1	A	47	ALA	2.6
1	A	272	VAL	2.6
1	A	613	HIS	2.6
1	A	314	ALA	2.5
1	A	390	LEU	2.5
1	A	309	MET	2.5
1	A	372	GLY	2.5
1	A	364	VAL	2.5
1	A	319	HIS	2.5
1	A	425	LEU	2.5
1	A	318	THR	2.4
1	A	389	ALA	2.4
1	A	583	ASP	2.4
1	A	375	ALA	2.4
1	A	630	ALA	2.4
1	A	344	ALA	2.3
1	A	62	GLY	2.3
1	A	342	SER	2.3
1	A	335	MET	2.3
1	A	34	ASP	2.2
1	A	373	SER	2.2
1	A	402	ARG	2.2
1	A	530	LEU	2.2
1	A	641	TYR	2.2
1	A	627	GLU	2.2
1	A	422	ILE	2.2
1	A	616	GLU	2.2
1	A	313	GLY	2.2
1	A	617	ASP	2.2
1	A	376	GLY	2.1
1	A	185	GLU	2.1
1	A	236	LYS	2.1
1	A	365	LEU	2.1
1	A	349	ALA	2.1
1	A	67	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	311	VAL	2.0
1	A	499	ARG	2.0
1	A	337	GLY	2.0
1	A	44	ASN	2.0
1	A	429	VAL	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](#)

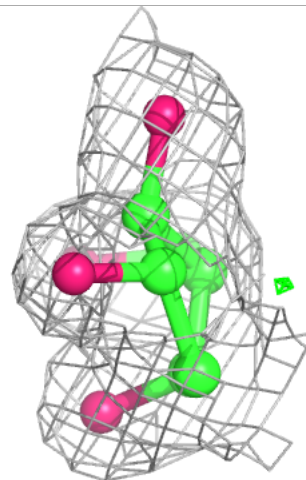
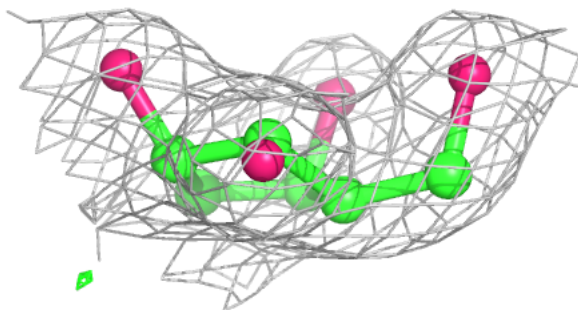
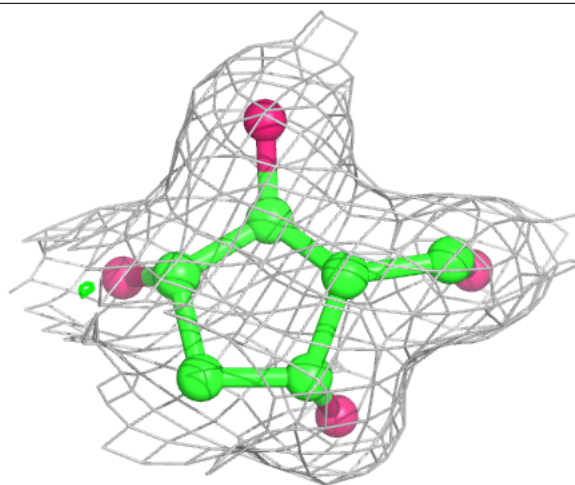
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	K	A	703	1/1	0.94	0.26	60,60,60,60	0
3	FE0	A	702	10/10	0.95	0.12	35,37,39,40	0
2	ZN	A	701	1/1	0.99	0.09	36,36,36,36	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.

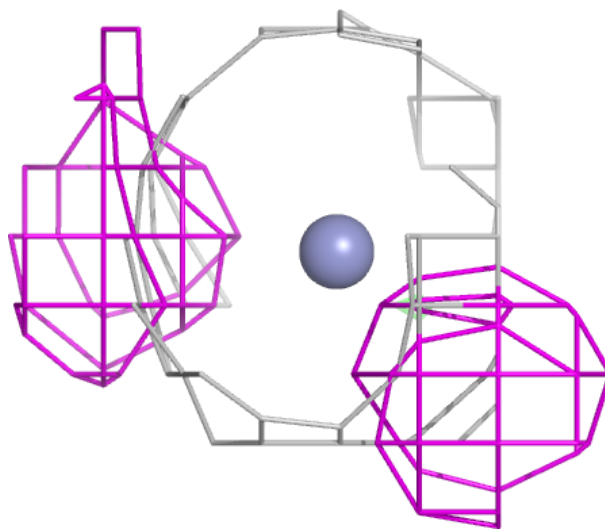
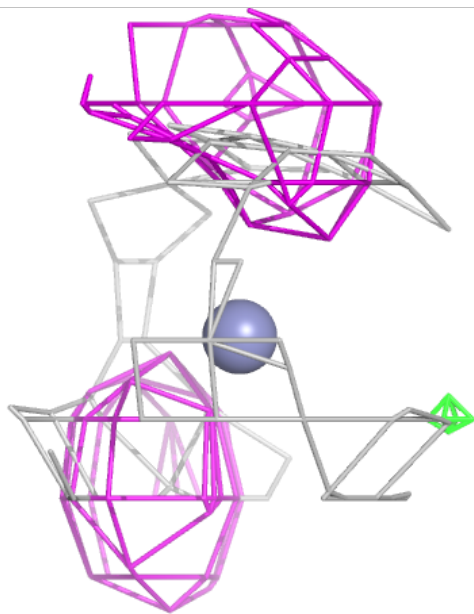
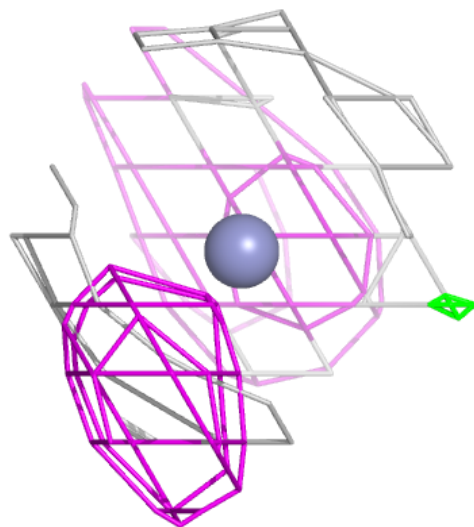
**Electron density around FE0 A 702:**

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



**Electron density around ZN A 701:**

$2mF_o-DF_c$  (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.