



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:41 PM UTC

PDB ID : 9FVU / pdb\_00009fvu  
Title : Aspartyl/Asparaginyl beta-hydroxylase (AspH) in complex with Fe, 2-oxoglutarate, thiocyanate and Factor X derived peptide fragment  
Authors : Brasnett, A.; de Munnik, M.; Brewitz, L.; Rabe, P.; Schofield, C.J.  
Deposited on : 2024-06-28  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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 Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

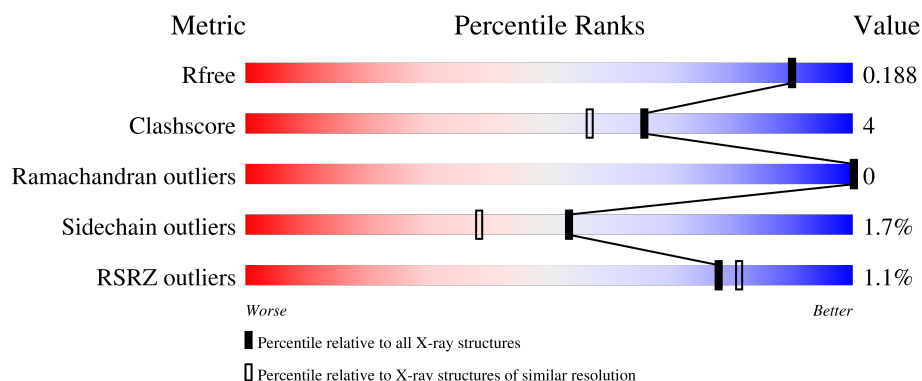
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	758	
2	B	39	

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
5	PEG	A	810	-	-	X	-
6	SCN	B	201[A]	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4097 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 Aspartyl/asparaginyl beta-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	4	0
			3447	2194	607	634	12			

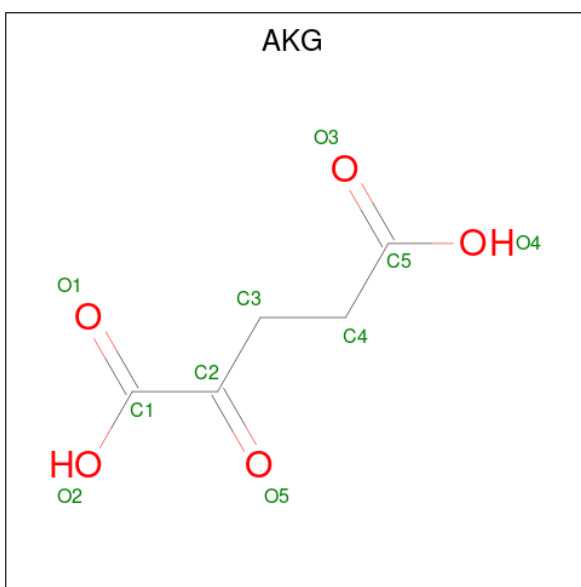
- Molecule 2 is a protein called Factor X light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	S	0	1	0
			132	80	23	27	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	90	SER	CYS	engineered mutation	UNP P00742
B	95	SER	CYS	engineered mutation	UNP P00742
B	103	ASN	ASP	conflict	UNP P00742
B	112	SER	CYS	engineered mutation	UNP P00742
B	121	SER	CYS	engineered mutation	UNP P00742

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

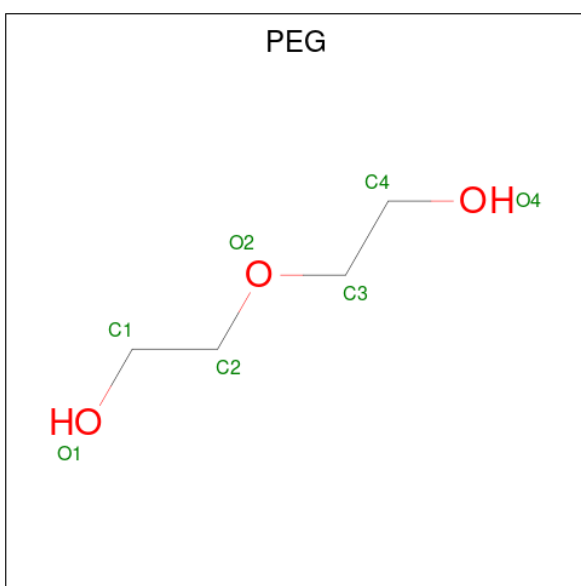


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

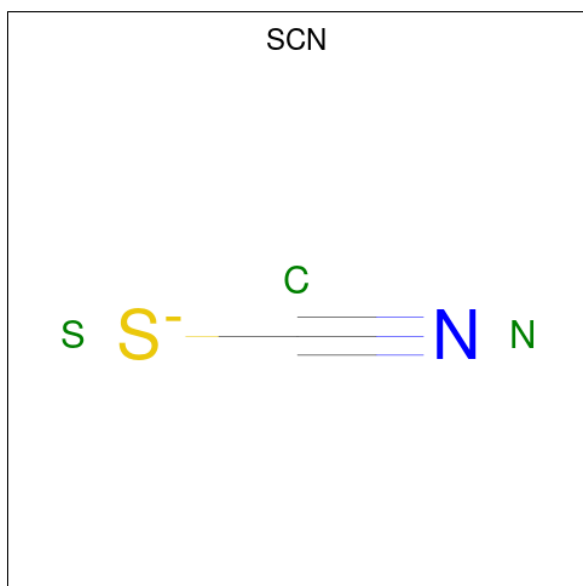
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



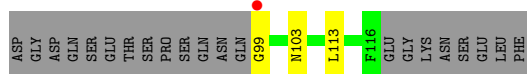
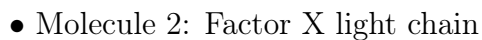
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	S	0	1
			3	1	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	439	Total 439	O 439	0	1
7	B	12	Total 12	O 12	0	0



- Molecule 1: Aspartyl/asparaginyl beta-hydroxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.64Å 85.89Å 123.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.08 – 1.70 46.08 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.08-1.70) 99.9 (46.08-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.173 , 0.187 0.174 , 0.188	Depositor DCC
$R_{free}$ test set	2000 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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: SCN, FE, AKG, PEG

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	0.54	0/3529	0.77	1/4772 (0.0%)
2	B	0.34	0/133	0.37	0/176
All	All	0.53	0/3662	0.76	1/4948 (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	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	386	ASP	CA-CB-CG	5.22	117.82	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	ARG	Sidechain
1	A	399	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	3447	0	3351	24	0
2	B	132	0	114	3	0
3	A	10	0	4	2	0
4	A	1	0	0	0	0
5	A	53	0	75	6	0
6	B	3	0	0	2	0
7	A	439	0	0	6	0
7	B	12	0	0	1	0
All	All	4097	0	3544	27	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 4.

The worst 5 of 27 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:701:LYS:NZ	5:A:810:PEG:H22	1.68	1.08
7:A:1235:HOH:O	2:B:113:LEU:CB	2.19	0.90
1:A:701:LYS:HZ3	5:A:810:PEG:H22	1.39	0.83
1:A:712:GLU:CD	7:A:901:HOH:O	2.28	0.76
1:A:652:GLU:HG3	7:A:1249:HOH:O	1.89	0.73

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	Percentiles	
1	A	431/758 (57%)	427 (99%)	4 (1%)	0	100	100
2	B	17/39 (44%)	17 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	448/797 (56%)	444 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	354/661 (54%)	348 (98%)	6 (2%)	53	38
2	B	13/33 (39%)	13 (100%)	0	100	100
All	All	367/694 (53%)	361 (98%)	6 (2%)	53	41

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	479	GLU
1	A	680	THR
1	A	729	GLN
1	A	370	LYS
1	A	350	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	A	435	HIS
1	A	561	GLN
1	A	566	ASN
1	A	671	HIS

### 5.3.3 RNA ⓘ

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z  > 2$
5	PEG	A	804	-	6,6,6	0.11	0	5,5,5	0.07	0
5	PEG	A	805	-	3,3,6	0.14	0	2,2,5	0.22	0
5	PEG	A	810	-	6,6,6	0.14	0	5,5,5	0.11	0
3	AKG	A	801	4	9,9,9	4.96	3 (33%)	11,11,11	1.79	3 (27%)
6	SCN	B	201[A]	4	1,2,2	0.76	0	0,1,1	-	-
5	PEG	A	803	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PEG	A	808	-	6,6,6	0.13	0	5,5,5	0.12	0
5	PEG	A	807	-	6,6,6	0.11	0	5,5,5	0.10	0
5	PEG	A	806	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PEG	A	809	-	6,6,6	0.12	0	5,5,5	0.08	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
5	PEG	A	804	-	-	2/4/4/4	-
5	PEG	A	805	-	-	1/1/1/4	-
5	PEG	A	810	-	-	3/4/4/4	-
3	AKG	A	801	4	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	803	-	-	3/4/4/4	-
5	PEG	A	808	-	-	2/4/4/4	-
5	PEG	A	807	-	-	1/4/4/4	-
5	PEG	A	806	-	-	0/4/4/4	-
5	PEG	A	809	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	AKG	C2-C1	-14.40	1.31	1.53
3	A	801	AKG	O2-C1	-2.92	1.22	1.30
3	A	801	AKG	O4-C5	-2.05	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	AKG	C3-C2-C1	3.77	122.27	115.86
3	A	801	AKG	O1-C1-C2	-2.57	118.61	121.81
3	A	801	AKG	O2-C1-C2	2.18	119.65	113.59

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	810	PEG	O1-C1-C2-O2
5	A	804	PEG	O2-C3-C4-O4
5	A	809	PEG	O1-C1-C2-O2
5	A	803	PEG	O1-C1-C2-O2
5	A	805	PEG	O1-C1-C2-O2

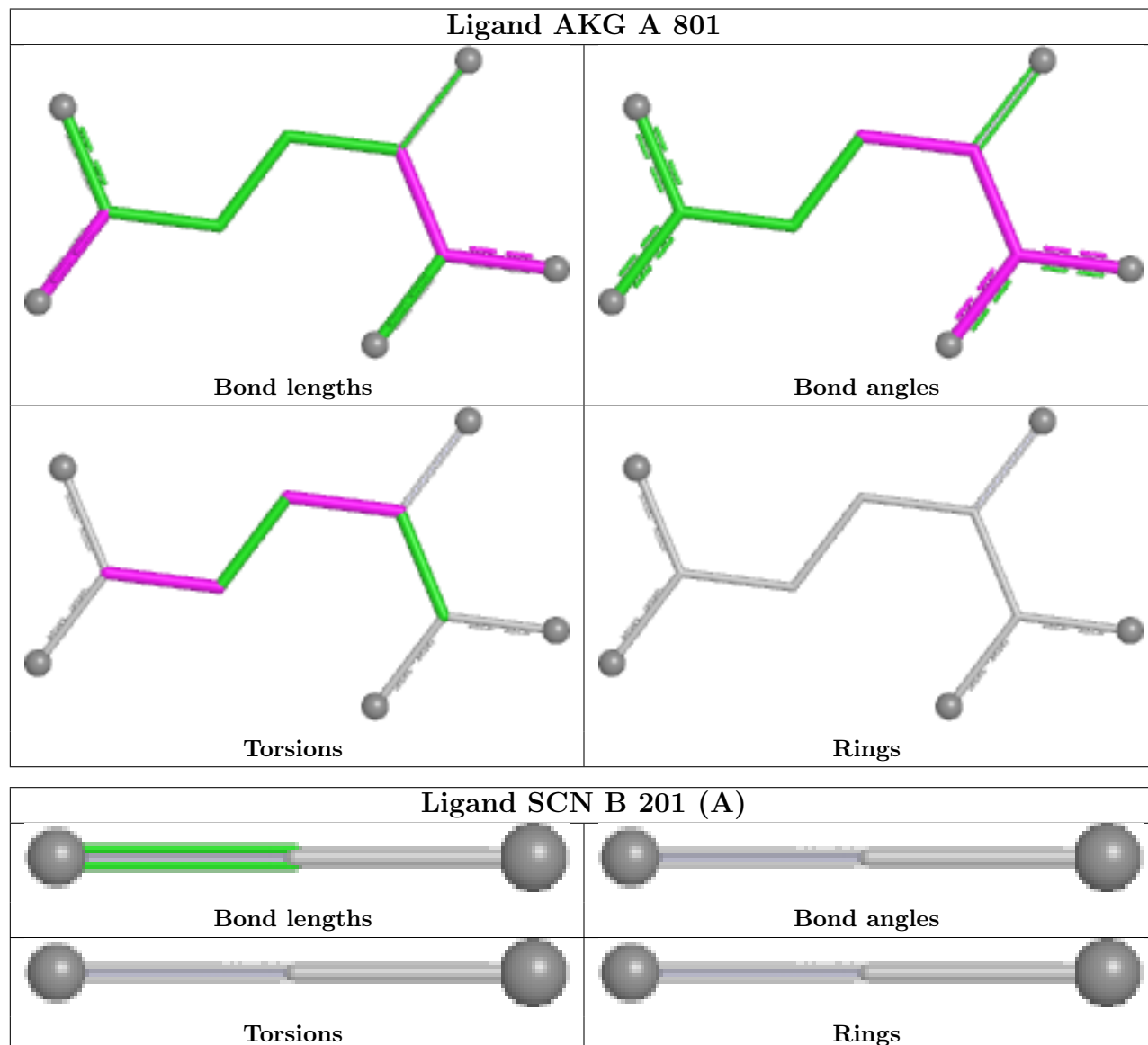
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	810	PEG	6	0
3	A	801	AKG	2	0
6	B	201[A]	SCN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	429/758 (56%)	-0.11	4 (0%) 81 83	11, 27, 43, 63	4 (0%)
2	B	18/39 (46%)	0.42	1 (5%) 30 33	14, 29, 46, 51	1 (5%)
All	All	447/797 (56%)	-0.09	5 (1%) 78 81	11, 27, 43, 63	5 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	ILE	2.5
1	A	544	TYR	2.3
1	A	330	LYS	2.2
1	A	549	LEU	2.2
2	B	99	GLY	2.2

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

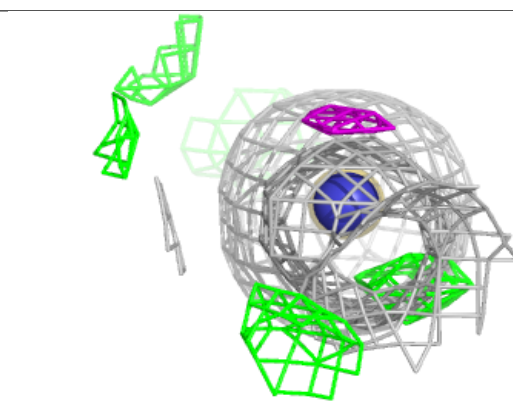
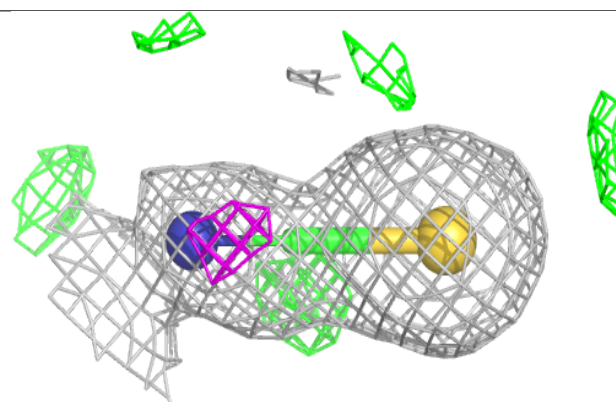
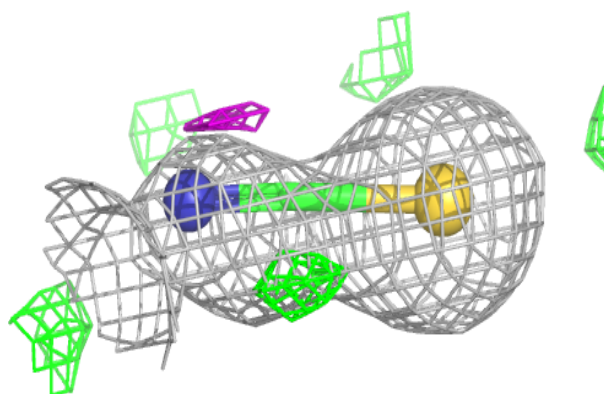
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
5	PEG	A	809	7/7	0.70	0.20	45,60,64,68	0
5	PEG	A	803	7/7	0.73	0.16	52,54,61,61	0
5	PEG	A	808	7/7	0.82	0.15	34,41,47,55	0
5	PEG	A	807	7/7	0.83	0.13	45,47,54,54	0
5	PEG	A	804	7/7	0.84	0.15	40,46,59,62	0
5	PEG	A	806	7/7	0.86	0.37	41,47,48,50	7
5	PEG	A	810	7/7	0.86	0.18	46,53,56,65	0
5	PEG	A	805	4/7	0.88	0.10	54,55,57,58	0
6	SCN	B	201[A]	3/3	0.95	0.12	22,22,24,27	3
3	AKG	A	801	10/10	0.96	0.06	17,19,22,22	0
4	FE	A	802	1/1	1.00	0.02	20,20,20,20	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.

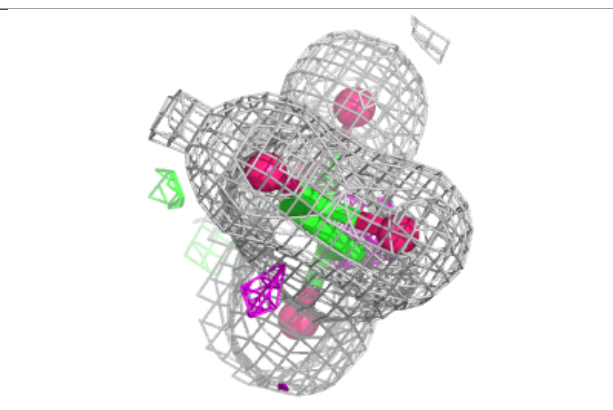
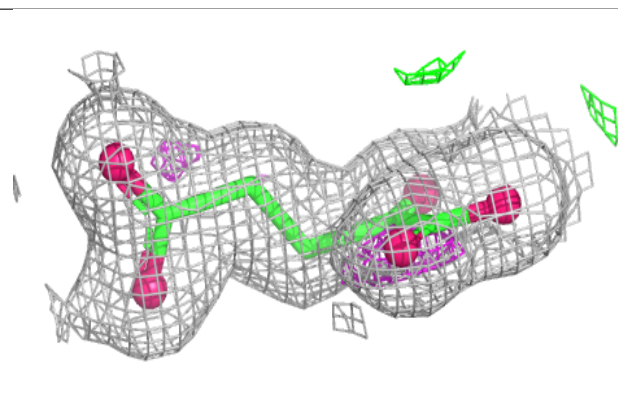
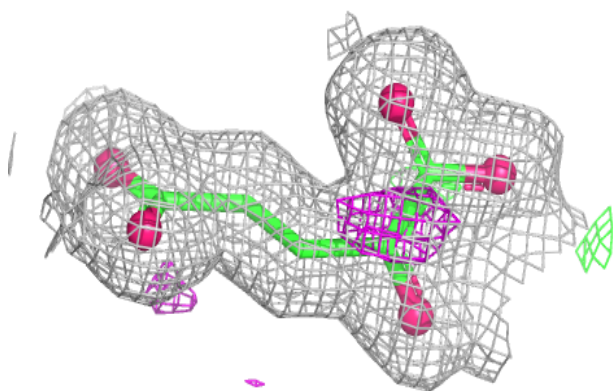
**Electron density around SCN B 201 (A):**

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



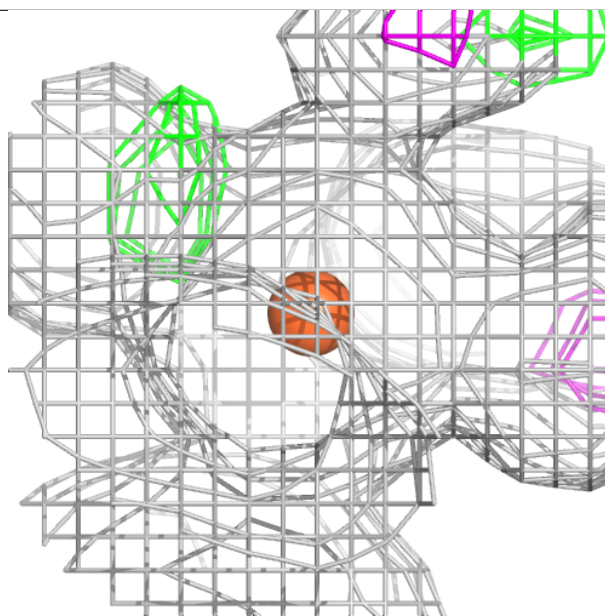
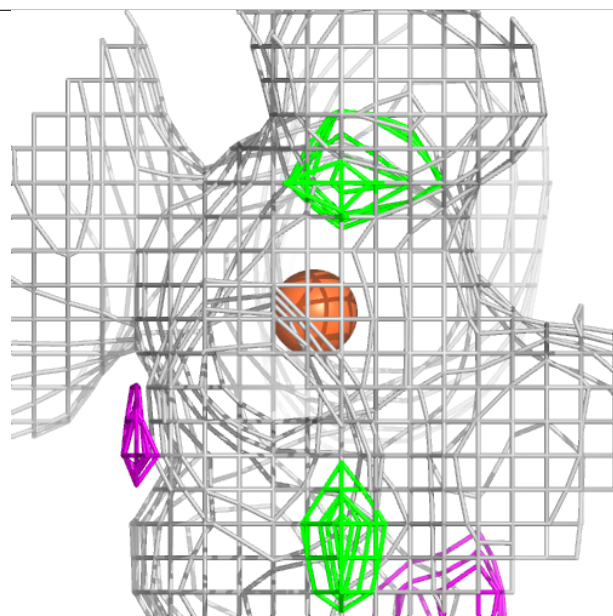
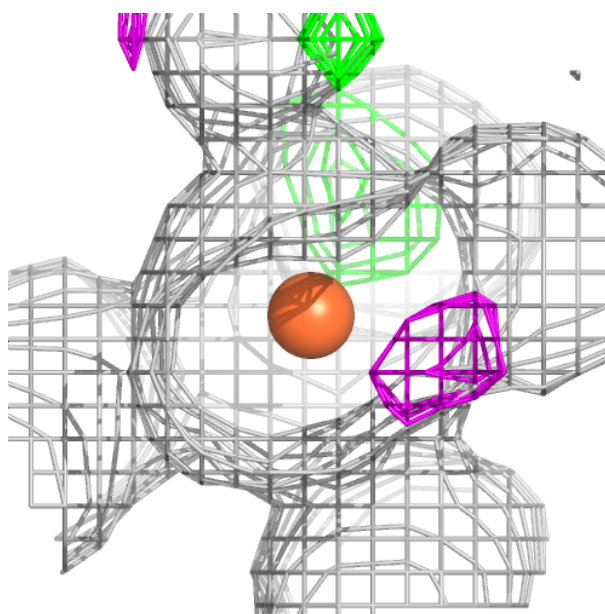
**Electron density around AKG A 801:**

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



**Electron density around FE A 802:**

$2mF_o-DF_c$  (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.