



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2025 – 10:08 AM EDT

PDB ID : 9BFA / pdb\_00009bfa  
Title : BCAT mutant  
Authors : Dong, M.  
Deposited on : 2024-04-17  
Resolution : 1.79 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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.43.1

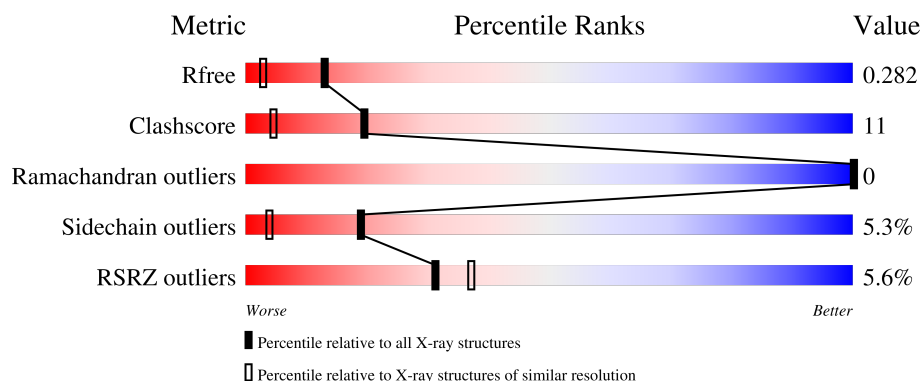
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	364	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	B	364	<div> <div>4%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	E	364	<div> <div>7%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	F	364	<div> <div>7%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12375 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 Branched-chain-amino-acid aminotransferase, cytosolic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	P	S	0	1	0
			2890	1857	476	541	1	15			
1	B	363	Total	C	N	O	P	S	0	0	0
			2885	1854	477	538	1	15			
1	E	364	Total	C	N	O	P	S	0	0	0
			2882	1853	474	539	1	15			
1	F	363	Total	C	N	O	P	S	0	0	0
			2885	1854	477	538	1	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	THR	conflict	UNP P54687
A	379	ARG	SER	conflict	UNP P54687
B	33	GLU	THR	conflict	UNP P54687
B	379	ARG	SER	conflict	UNP P54687
E	33	GLU	THR	conflict	UNP P54687
E	379	ARG	SER	conflict	UNP P54687
F	33	GLU	THR	conflict	UNP P54687
F	379	ARG	SER	conflict	UNP P54687

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mg	0	0
			3	3		

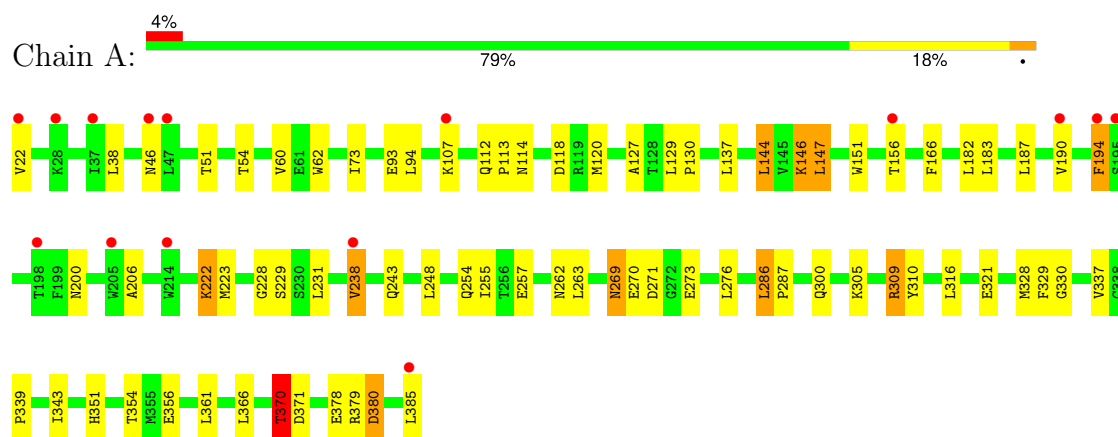
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	207	Total 207	O 207	0	0
3	B	183	Total 183	O 183	0	0
3	E	230	Total 230	O 230	0	0
3	F	210	Total 210	O 210	0	0

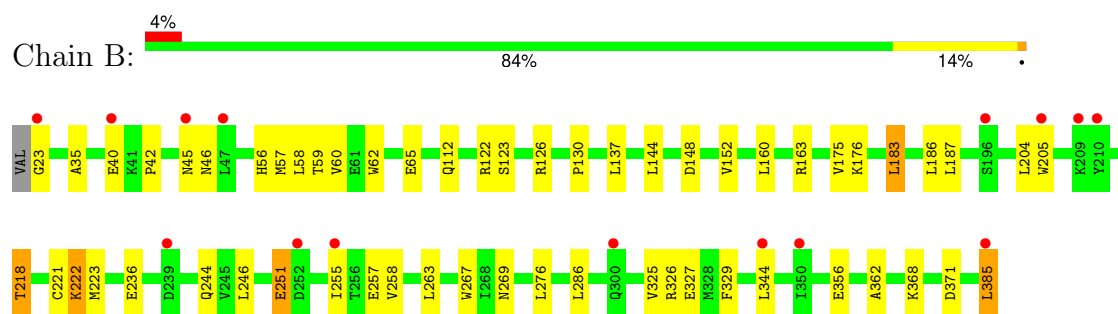
### 3 Residue-property plots [i](#)

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.

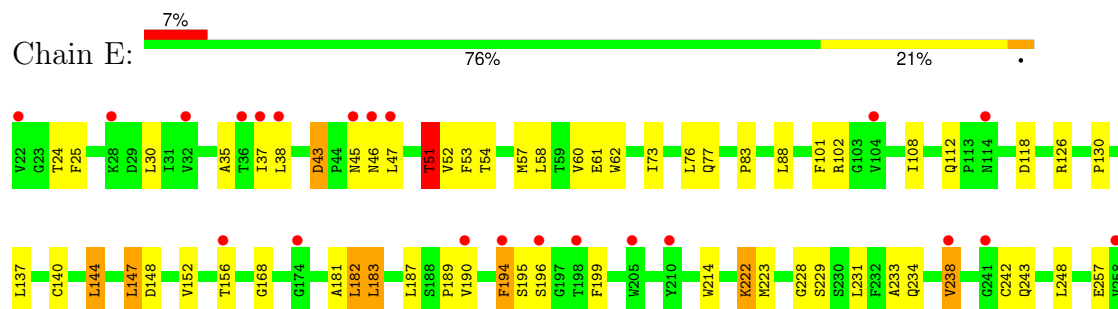
- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic



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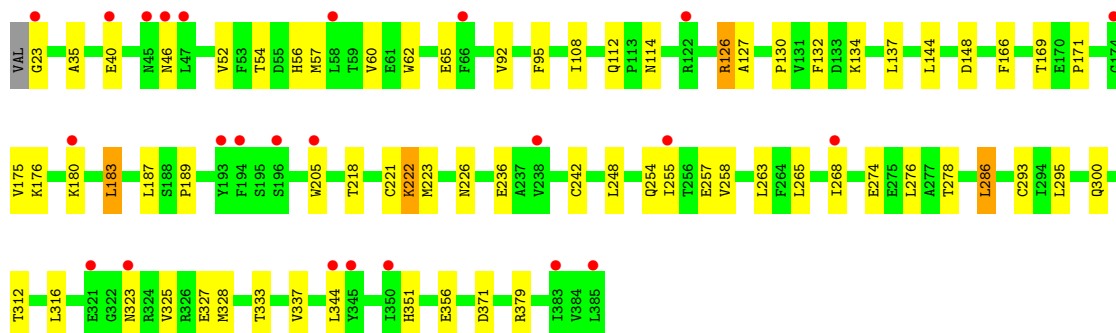
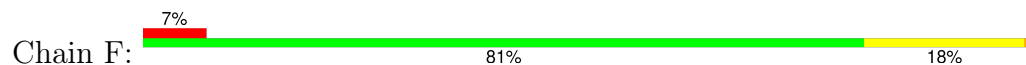


- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic





- Molecule 1: Branched-chain-amino-acid aminotransferase, cytosolic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.28Å 115.63Å 149.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.44 – 1.79 91.44 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.44-1.79) 99.4 (91.44-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.232 , 0.268 0.245 , 0.282	Depositor DCC
$R_{free}$ test set	8991 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 25.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7992e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: MG, LLP

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	0.59	0/2939	1.09	10/3999 (0.3%)
1	B	0.59	0/2934	1.07	5/3989 (0.1%)
1	E	0.59	0/2931	1.07	7/3988 (0.2%)
1	F	0.60	0/2934	1.06	7/3989 (0.2%)
All	All	0.59	0/11738	1.07	29/15965 (0.2%)

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	E	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	THR	CA-CB-OG1	-10.31	94.14	109.60
1	E	156	THR	CA-CB-OG1	-7.38	98.53	109.60
1	E	194	PHE	CB-CA-C	7.03	123.17	109.33
1	A	370	THR	CA-CB-OG1	-7.01	99.09	109.60
1	A	194	PHE	CB-CA-C	6.84	122.81	109.33

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	E	126	ARG	Sidechain
1	F	126	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	2890	0	2840	64	0
1	B	2885	0	2847	50	0
1	E	2882	0	2835	84	0
1	F	2885	0	2846	63	0
2	B	3	0	0	0	0
3	A	207	0	0	35	0
3	B	183	0	0	29	0
3	E	230	0	0	56	0
3	F	210	0	0	41	0
All	All	12375	0	11368	261	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 11.

The worst 5 of 261 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:337:VAL:HB	3:A:623:HOH:O	1.48	1.13
1:F:268:ILE:HG13	3:F:672:HOH:O	1.61	0.99
1:B:152:VAL:HG13	3:B:503:HOH:O	1.60	0.99
1:E:102:ARG:HG3	3:E:511:HOH:O	1.66	0.96
1:E:339:PRO:HD3	3:E:505:HOH:O	1.69	0.92

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	362/364 (100%)	350 (97%)	12 (3%)	0	100	100
1	B	360/364 (99%)	350 (97%)	10 (3%)	0	100	100
1	E	361/364 (99%)	348 (96%)	13 (4%)	0	100	100
1	F	360/364 (99%)	351 (98%)	9 (2%)	0	100	100
All	All	1443/1456 (99%)	1399 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	314/316 (99%)	294 (94%)	20 (6%)	14	2
1	B	314/316 (99%)	300 (96%)	14 (4%)	23	6
1	E	313/316 (99%)	292 (93%)	21 (7%)	13	2
1	F	314/316 (99%)	303 (96%)	11 (4%)	31	11
All	All	1255/1264 (99%)	1189 (95%)	66 (5%)	19	4

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	112	GLN
1	F	171	PRO
1	F	356	GLU

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Mol	Chain	Res	Type
1	B	112	GLN
1	B	65	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	226	ASN
1	E	351	HIS
1	E	300	GLN
1	F	45	ASN
1	B	56	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	E	222	1	23,24,25	0.60	0	25,32,34	1.55	5 (20%)
1	LLP	F	222	1	23,24,25	0.55	0	25,32,34	1.47	5 (20%)
1	LLP	A	222	1	23,24,25	0.61	0	25,32,34	1.36	4 (16%)
1	LLP	B	222	1	23,24,25	0.62	0	25,32,34	1.47	6 (24%)

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
1	LLP	E	222	1	-	4/16/17/19	0/1/1/1
1	LLP	F	222	1	-	4/16/17/19	0/1/1/1
1	LLP	A	222	1	-	4/16/17/19	0/1/1/1
1	LLP	B	222	1	-	3/16/17/19	0/1/1/1

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	LLP	OP4-C5'-C5	3.77	116.42	109.36
1	E	222	LLP	OP4-C5'-C5	3.59	116.08	109.36
1	F	222	LLP	CD-CE-NZ	3.50	120.11	110.83
1	E	222	LLP	C5-C4-C4'	3.44	126.78	121.47
1	A	222	LLP	C5-C4-C4'	3.28	126.53	121.47

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	222	LLP	N-CA-CB-CG
1	A	222	LLP	C-CA-CB-CG
1	B	222	LLP	N-CA-CB-CG
1	B	222	LLP	C-CA-CB-CG
1	E	222	LLP	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	222	LLP	2	0
1	F	222	LLP	4	0
1	A	222	LLP	2	0
1	B	222	LLP	2	0

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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	363/364 (99%)	0.36	15 (4%) 42 48	14, 30, 50, 88	1 (0%)
1	B	362/364 (99%)	0.36	15 (4%) 42 48	20, 31, 50, 62	0
1	E	363/364 (99%)	0.37	27 (7%) 22 26	21, 30, 51, 87	0
1	F	362/364 (99%)	0.56	24 (6%) 26 31	20, 33, 52, 69	0
All	All	1450/1456 (99%)	0.41	81 (5%) 31 37	14, 31, 51, 88	1 (0%)

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	PHE	9.0
1	A	22	VAL	8.8
1	E	194	PHE	7.6
1	E	22	VAL	6.9
1	F	385	LEU	4.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	F	222	24/25	0.97	0.08	24,32,36,38	0
1	LLP	B	222	24/25	0.98	0.08	22,27,30,33	0
1	LLP	E	222	24/25	0.98	0.06	22,26,29,30	0
1	LLP	A	222	24/25	0.98	0.06	21,26,28,30	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

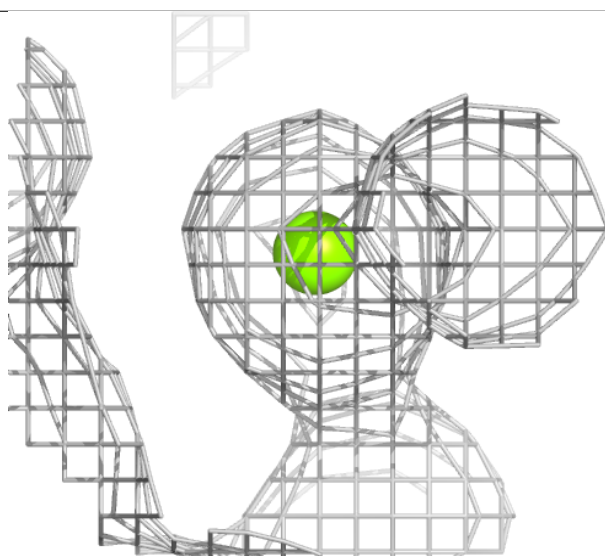
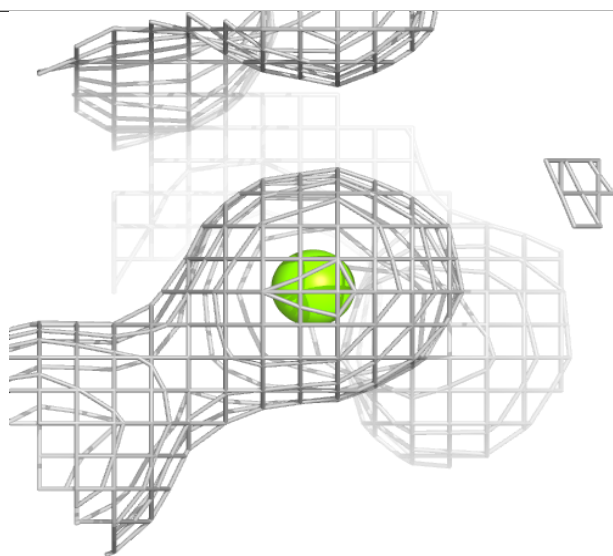
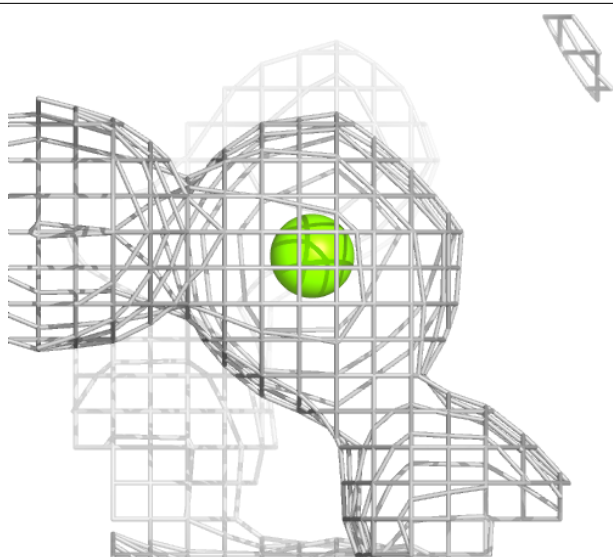
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	MG	B	402	1/1	0.97	0.09	43,43,43,43	0
2	MG	B	401	1/1	0.98	0.13	39,39,39,39	0
2	MG	B	403	1/1	0.98	0.19	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 MG B 402:**

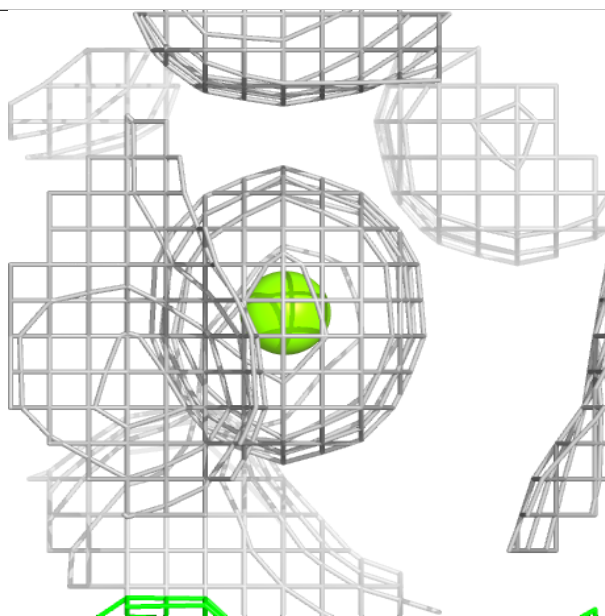
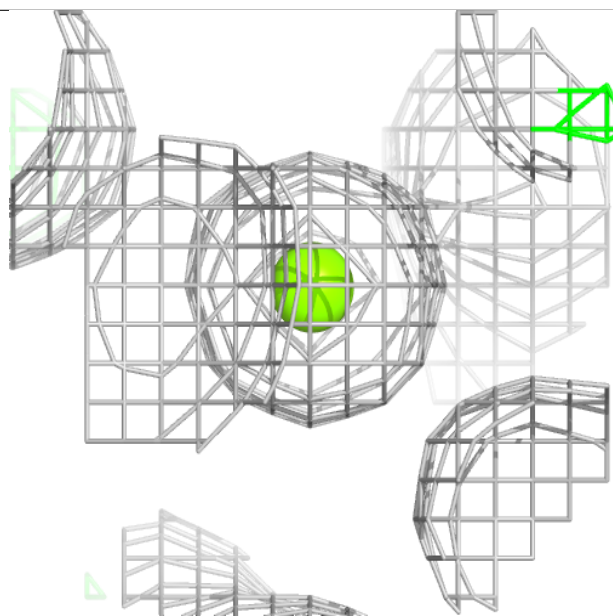
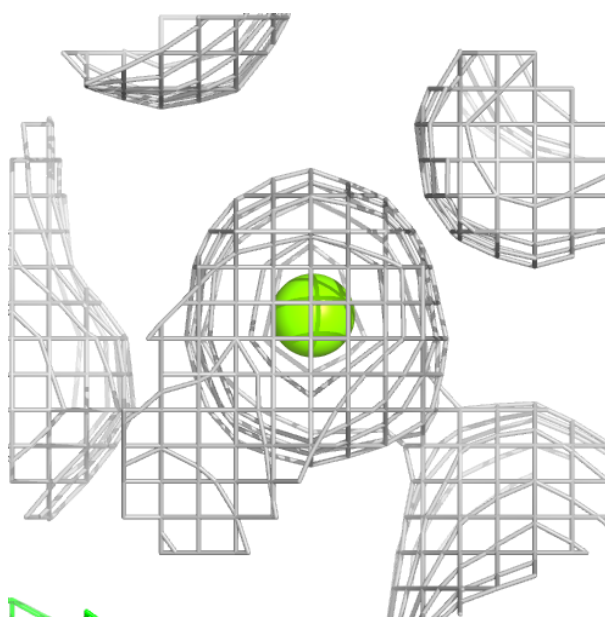
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





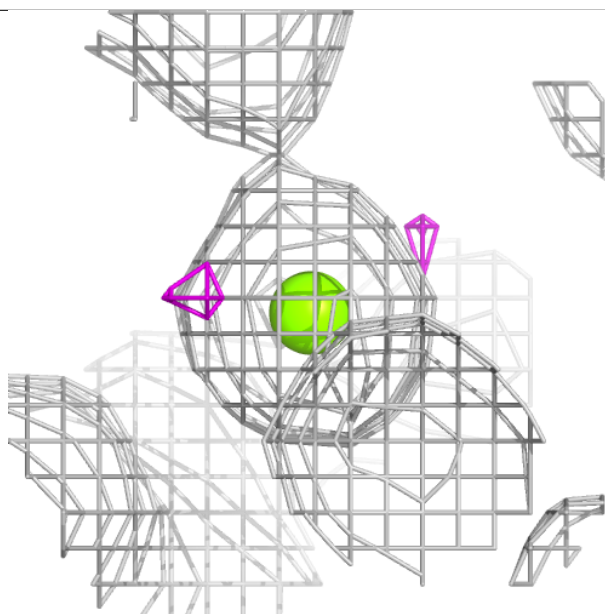
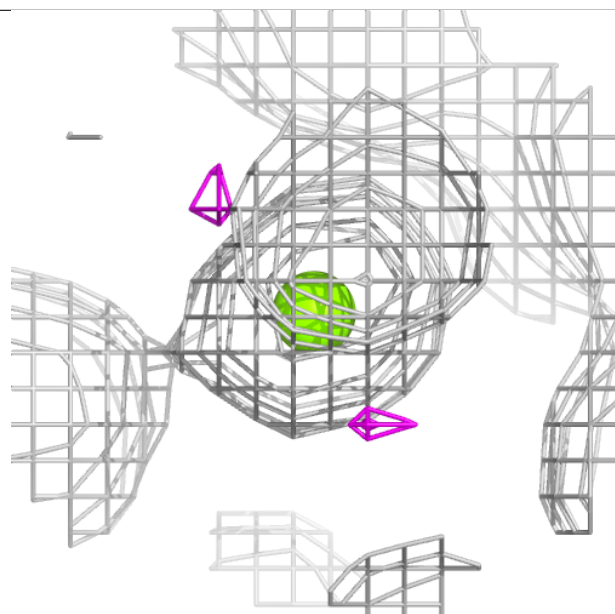
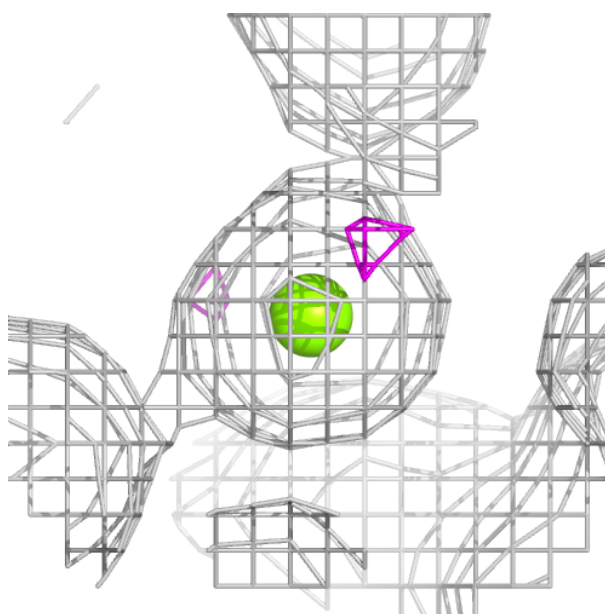
**Electron density around MG B 401:**

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



**Electron density around MG B 403:**

$2mF_o-DF_c$  (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.