



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:36 AM GMT

PDB ID : 2B3H  
Title : Crystal structure of Human Methionine Aminopeptidase Type I with a third cobalt in the active site  
Authors : Addlagatta, A.; Hu, X.; Liu, J.O.; Matthews, B.W.  
Deposited on : 2005-09-20  
Resolution : 1.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

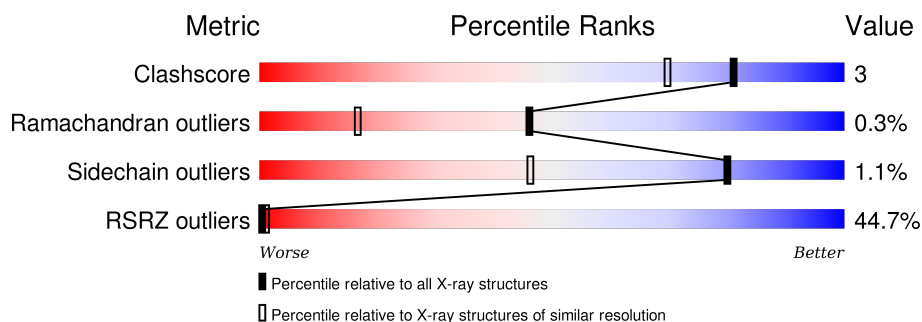
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.10 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))
Clashscore	102246	1055 (1.14-1.06)
Ramachandran outliers	100387	1016 (1.14-1.06)
Sidechain outliers	100360	1014 (1.14-1.06)
RSRZ outliers	91569	1009 (1.14-1.06)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	329	<div> <div>41%</div> <div>77%</div> <div>14%</div> <div>8%</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
5	GOL	A	470[A]	-	-	-	X
5	GOL	A	470[B]	-	-	-	X
5	GOL	A	471	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2981 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 Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2446	1540	438	445	23	0	13	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	MET	-	CLONING ARTIFACT	UNP P53582
A	66	GLY	-	CLONING ARTIFACT	UNP P53582
A	67	SER	-	CLONING ARTIFACT	UNP P53582
A	68	SER	-	CLONING ARTIFACT	UNP P53582
A	69	HIS	-	EXPRESSION TAG	UNP P53582
A	70	HIS	-	EXPRESSION TAG	UNP P53582
A	71	HIS	-	EXPRESSION TAG	UNP P53582
A	72	HIS	-	EXPRESSION TAG	UNP P53582
A	73	HIS	-	EXPRESSION TAG	UNP P53582
A	74	HIS	-	EXPRESSION TAG	UNP P53582
A	75	SER	-	CLONING ARTIFACT	UNP P53582
A	76	SER	-	CLONING ARTIFACT	UNP P53582
A	77	GLY	-	CLONING ARTIFACT	UNP P53582
A	78	LEU	-	CLONING ARTIFACT	UNP P53582
A	79	VAL	-	CLONING ARTIFACT	UNP P53582
A	80	PRO	-	CLONING ARTIFACT	UNP P53582
A	81	ARG	-	CLONING ARTIFACT	UNP P53582
A	82	GLY	-	CLONING ARTIFACT	UNP P53582
A	83	SER	-	CLONING ARTIFACT	UNP P53582
A	84	HIS	-	CLONING ARTIFACT	UNP P53582
A	85	MET	-	CLONING ARTIFACT	UNP P53582
A	86	LEU	-	CLONING ARTIFACT	UNP P53582
A	87	GLU	-	CLONING ARTIFACT	UNP P53582
A	88	ASP	-	CLONING ARTIFACT	UNP P53582
A	89	PRO	-	CLONING ARTIFACT	UNP P53582

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

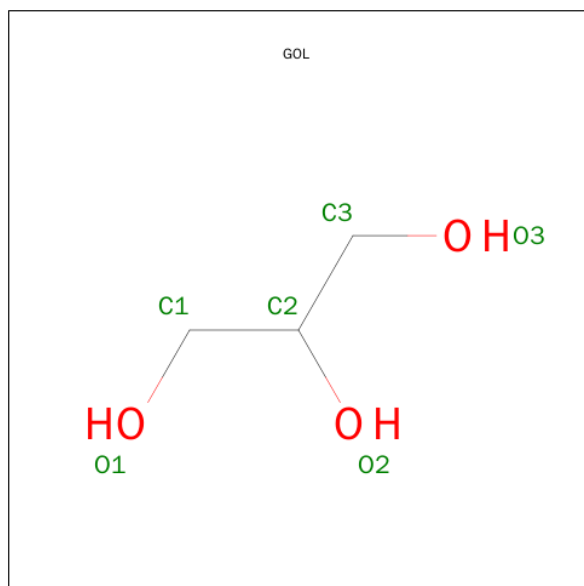
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

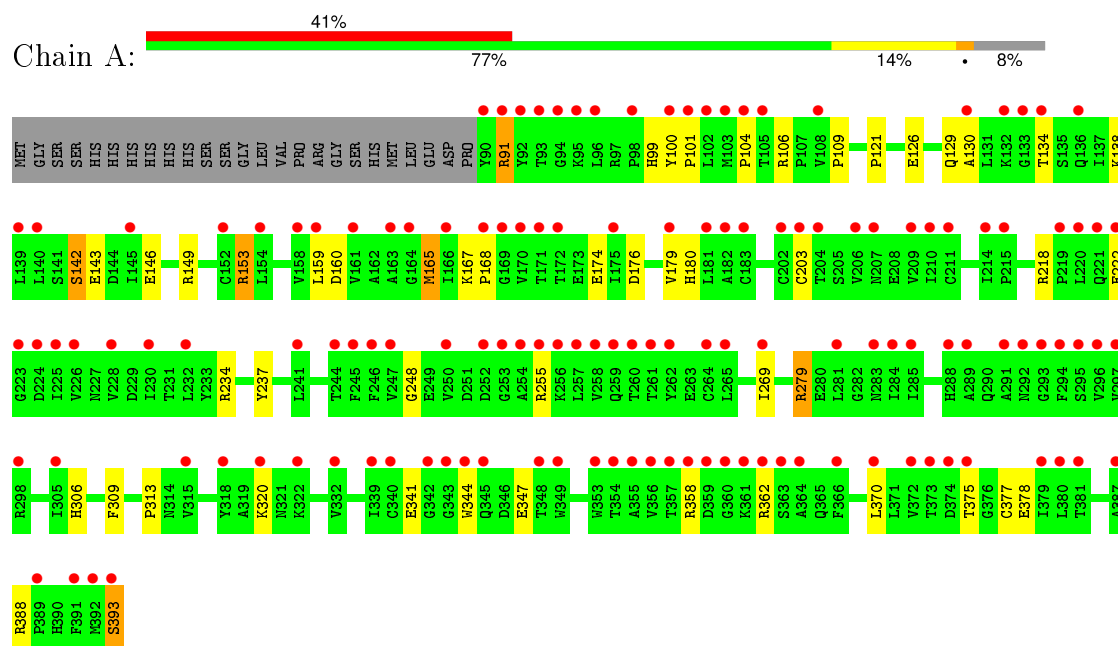
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	511	Total 511	O 511	0	0

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Methionine aminopeptidase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.29Å 77.30Å 48.34Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10 18.91 – 1.10	Depositor EDS
% Data completeness (in resolution range)	91.6 (20.00-1.10) 91.7 (18.91-1.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 1.10Å)	Xtriage
Refinement program	SHELXL	Depositor
R, $R_{free}$	0.101 , 0.131 0.290 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	10.1	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.1	EDS
Estimated twinning fraction	0.000 for l,k,-h 0.018 for h,-k,-l 0.014 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 255244 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, K, CO, CL

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	1.41	12/2562 (0.5%)	1.72	53/3473 (1.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	SER	C-OXT	28.58	1.77	1.23
1	A	143	GLU	CD-OE2	7.44	1.33	1.25
1	A	341	GLU	CB-CG	-7.26	1.38	1.52
1	A	121	PRO	C-O	6.94	1.37	1.23
1	A	341	GLU	CD-OE1	6.75	1.33	1.25
1	A	109	PRO	N-CD	-5.94	1.39	1.47
1	A	234	ARG	NE-CZ	-5.89	1.25	1.33
1	A	142	SER	CA-CB	5.77	1.61	1.52
1	A	104	PRO	N-CD	-5.67	1.40	1.47
1	A	347	GLU	CD-OE1	5.56	1.31	1.25
1	A	168	PRO	N-CD	-5.43	1.40	1.47
1	A	378	GLU	CD-OE2	-5.42	1.19	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91[A]	ARG	CD-NE-CZ	22.11	154.55	123.60
1	A	91[B]	ARG	CD-NE-CZ	22.11	154.55	123.60
1	A	153	ARG	NE-CZ-NH1	17.02	128.81	120.30
1	A	255	ARG	NE-CZ-NH2	16.75	128.68	120.30
1	A	234	ARG	CD-NE-CZ	16.05	146.08	123.60
1	A	149	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	A	377[A]	CYS	N-CA-CB	-10.20	92.23	110.60
1	A	377[B]	CYS	N-CA-CB	-10.20	92.23	110.60
1	A	344	TRP	CE3-CZ3-CH2	-9.57	110.67	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	A	165[A]	MET	CA-CB-CG	-9.27	97.54	113.30
1	A	165[B]	MET	CA-CB-CG	-9.27	97.54	113.30
1	A	153	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	A	393	SER	CA-C-O	-8.47	102.32	120.10
1	A	279[A]	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	A	279[B]	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	A	255	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	A	121	PRO	O-C-N	-8.25	109.50	122.70
1	A	393	SER	CB-CA-C	7.77	124.86	110.10
1	A	104	PRO	N-CD-CG	7.73	114.79	103.20
1	A	174	GLU	OE1-CD-OE2	-7.66	114.11	123.30
1	A	143	GLU	CB-CG-CD	7.55	134.60	114.20
1	A	134	THR	CA-CB-CG2	-7.38	102.06	112.40
1	A	393	SER	N-CA-C	-7.21	91.53	111.00
1	A	91[A]	ARG	CB-CG-CD	7.20	130.32	111.60
1	A	91[B]	ARG	CB-CG-CD	7.20	130.32	111.60
1	A	126	GLU	CG-CD-OE2	6.87	132.03	118.30
1	A	375	THR	CA-CB-OG1	-6.75	94.83	109.00
1	A	149	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	104	PRO	O-C-N	-6.55	112.21	122.70
1	A	174	GLU	CG-CD-OE1	6.47	131.24	118.30
1	A	313	PRO	N-CD-CG	6.41	112.81	103.20
1	A	218	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	138	LYS	CG-CD-CE	6.25	130.65	111.90
1	A	146	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	A	388	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	A	234	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	A	237	TYR	CB-CG-CD1	5.94	124.56	121.00
1	A	160	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	358	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	A	362	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	168	PRO	O-C-N	-5.43	113.97	123.20
1	A	104	PRO	CA-C-O	5.39	133.14	120.20
1	A	91[A]	ARG	CG-CD-NE	5.35	123.03	111.80
1	A	91[B]	ARG	CG-CD-NE	5.35	123.03	111.80
1	A	121	PRO	CA-C-N	5.33	128.92	117.20
1	A	222	GLU	OE1-CD-OE2	5.32	129.69	123.30
1	A	91[A]	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	91[B]	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	344	TRP	CZ3-CH2-CZ2	5.02	127.63	121.60
1	A	159[A]	LEU	CD1-CG-CD2	-5.02	95.44	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159[B]	LEU	CD1-CG-CD2	-5.02	95.44	110.50
1	A	126	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2446	0	2405	15	1
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	1	0
5	A	18	0	22	1	0
6	A	511	0	0	8	0
All	All	2981	0	2427	16	1

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 (16) 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:393:SER:C	1:A:393:SER:OXT	1.77	1.21
4:A:406:CL:CL	6:A:510:HOH:O	2.12	1.03
1:A:393:SER:OXT	1:A:393:SER:O	1.98	0.81
1:A:99:HIS:HD2	6:A:952:HOH:O	1.91	0.53
1:A:165[B]:MET:SD	6:A:918:HOH:O	2.61	0.47
1:A:153:ARG:NH1	6:A:754:HOH:O	2.47	0.47
1:A:176:ASP:HA	1:A:179[B]:VAL:HG22	1.95	0.47
1:A:203:CYS:SG	5:A:471:GOL:H31	2.56	0.46
1:A:320:LYS:NZ	6:A:1009:HOH:O	2.48	0.45
1:A:269:ILE:HG12	1:A:370[A]:LEU:HD11	1.99	0.45
1:A:248:GLY:HA2	6:A:973:HOH:O	2.17	0.44
1:A:176:ASP:O	1:A:179[B]:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:HB3	1:A:101:PRO:HA	2.02	0.42
1:A:129:GLN:NE2	6:A:974:HOH:O	2.52	0.42
1:A:279[B]:ARG:CZ	6:A:892:HOH:O	2.68	0.41
1:A:179[B]:VAL:HG23	1:A:180:HIS:N	2.37	0.40

All (1) 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:130:ALA:O	1:A:167:LYS:NZ[1_554]	2.14	0.06

## 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	315/329 (96%)	309 (98%)	5 (2%)	1 (0%)	46 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	HIS

### 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	274/283 (97%)	270 (98%)	4 (2%)	72 33

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91[A]	ARG
1	A	91[B]	ARG
1	A	142	SER
1	A	309	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	197	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	GOL	A	470[A]	-	5,5,5	1.26	1 (20%)	5,5,5	1.37	1 (20%)
5	GOL	A	470[B]	-	5,5,5	0.45	0	5,5,5	1.95	2 (40%)
5	GOL	A	471	2	5,5,5	1.43	1 (20%)	5,5,5	1.96	2 (40%)

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	GOL	A	470[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	A	470[B]	-	-	0/4/4/4	0/0/0/0
5	GOL	A	471	2	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	471	GOL	C3-C2	2.15	1.60	1.52
5	A	470[A]	GOL	O3-C3	2.32	1.52	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	471	GOL	O3-C3-C2	-2.96	95.85	110.18
5	A	470[B]	GOL	O1-C1-C2	-2.70	97.11	110.18
5	A	470[B]	GOL	C3-C2-C1	-2.22	102.41	111.12
5	A	470[A]	GOL	O2-C2-C3	2.12	118.35	108.65
5	A	471	GOL	C3-C2-C1	2.40	120.52	111.12

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
5	A	471	GOL	1	0

## 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 ⓘ

### 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	304/329 (92%)	1.97	136 (44%) 0 1	7, 14, 30, 45	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	5.3
1	A	293	GLY	5.1
1	A	246	PHE	4.7
1	A	349	TRP	4.6
1	A	291	ALA	4.6
1	A	294	PHE	4.4
1	A	247	VAL	4.3
1	A	92	TYR	4.3
1	A	225	ILE	4.3
1	A	257	LEU	4.3
1	A	91[A]	ARG	4.3
1	A	96	LEU	4.2
1	A	339	ILE	4.2
1	A	357	THR	4.0
1	A	366	PHE	3.9
1	A	356	VAL	3.9
1	A	340	CYS	3.9
1	A	93	THR	3.9
1	A	166	ILE	3.8
1	A	220	LEU	3.8
1	A	296	VAL	3.6
1	A	264	CYS	3.6
1	A	387	ALA	3.6
1	A	179[A]	VAL	3.6
1	A	221	GLN	3.5
1	A	344	TRP	3.5
1	A	252	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	100	TYR	3.5
1	A	223	GLY	3.5
1	A	170[A]	VAL	3.5
1	A	364	ALA	3.5
1	A	292	ASN	3.4
1	A	289	ALA	3.4
1	A	393	SER	3.4
1	A	297	VAL	3.3
1	A	226	VAL	3.3
1	A	343	GLY	3.3
1	A	285	ILE	3.3
1	A	222	GLU	3.3
1	A	169	GLY	3.2
1	A	214	ILE	3.2
1	A	211	CYS	3.2
1	A	261	THR	3.1
1	A	132	LYS	3.1
1	A	245	PHE	3.1
1	A	228	VAL	3.1
1	A	210	ILE	3.0
1	A	392[A]	MET	3.0
1	A	353	TRP	3.0
1	A	360	GLY	3.0
1	A	206	VAL	3.0
1	A	207	ASN	2.9
1	A	244	THR	2.9
1	A	342	GLY	2.9
1	A	375	THR	2.9
1	A	102	LEU	2.9
1	A	95	LYS	2.9
1	A	202	CYS	2.9
1	A	389	PRO	2.9
1	A	209	VAL	2.8
1	A	172	THR	2.8
1	A	101	PRO	2.8
1	A	355	ALA	2.8
1	A	175	ILE	2.8
1	A	133	GLY	2.8
1	A	254	ALA	2.8
1	A	159[A]	LEU	2.8
1	A	258	VAL	2.8
1	A	90	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	2.7
1	A	140	LEU	2.7
1	A	145	ILE	2.7
1	A	374	ASP	2.7
1	A	181	LEU	2.7
1	A	108	VAL	2.7
1	A	161	VAL	2.7
1	A	332	VAL	2.7
1	A	363	SER	2.6
1	A	203	CYS	2.6
1	A	265	LEU	2.6
1	A	158	VAL	2.6
1	A	345	GLN	2.5
1	A	372	VAL	2.6
1	A	391	PHE	2.5
1	A	134	THR	2.5
1	A	370[A]	LEU	2.5
1	A	381	THR	2.5
1	A	171	THR	2.5
1	A	283	ASN	2.5
1	A	359	ASP	2.5
1	A	204	THR	2.4
1	A	260	THR	2.4
1	A	98	PRO	2.4
1	A	105[A]	THR	2.4
1	A	358	ARG	2.4
1	A	168	PRO	2.4
1	A	232	LEU	2.4
1	A	152	CYS	2.4
1	A	259	GLN	2.4
1	A	262	TYR	2.4
1	A	373	THR	2.4
1	A	269	ILE	2.4
1	A	164	GLY	2.3
1	A	288	HIS	2.3
1	A	230	ILE	2.3
1	A	320	LYS	2.3
1	A	130	ALA	2.3
1	A	256	LYS	2.3
1	A	253	GLY	2.3
1	A	215	PRO	2.3
1	A	224	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	241	LEU	2.2
1	A	380	LEU	2.2
1	A	318	TYR	2.2
1	A	94	GLY	2.2
1	A	255	ARG	2.1
1	A	379	ILE	2.1
1	A	163	ALA	2.1
1	A	281	LEU	2.1
1	A	136	GLN	2.1
1	A	315	VAL	2.1
1	A	305	ILE	2.1
1	A	183[A]	CYS	2.1
1	A	322	LYS	2.1
1	A	362	ARG	2.1
1	A	284	ILE	2.1
1	A	298	ARG	2.1
1	A	219	PRO	2.1
1	A	295	SER	2.1
1	A	354	THR	2.1
1	A	154	LEU	2.0
1	A	104	PRO	2.0
1	A	182	ALA	2.0
1	A	361	LYS	2.0
1	A	348	THR	2.0
1	A	103	MET	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	471	6/6	0.64	0.23	12.25	20,27,37,38	0
5	GOL	A	470[A]	6/6	0.79	0.24	4.95	6,12,14,16	6
5	GOL	A	470[B]	6/6	0.79	0.24	4.61	10,12,13,13	6
4	CL	A	406	1/1	0.95	0.13	0.94	46,46,46,46	1
3	K	A	405	1/1	0.79	0.18	0.16	11,11,11,11	0
2	CO	A	401	1/1	0.93	0.11	-0.89	8,8,8,8	0
2	CO	A	402	1/1	0.92	0.12	-1.36	7,7,7,7	0
2	CO	A	403	1/1	0.91	0.12	-	10,10,10,10	1
2	CO	A	404	1/1	0.85	0.23	-	16,16,16,16	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.