



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 09:46 PM EDT

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

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>.

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 : 2.35
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) : 2.35

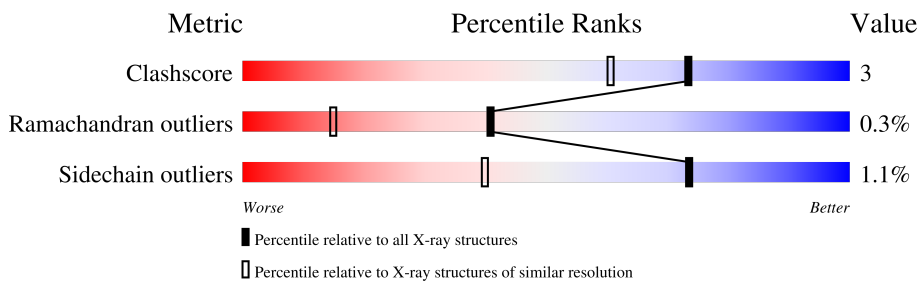
1 Overall quality at a glance

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	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	329	

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	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

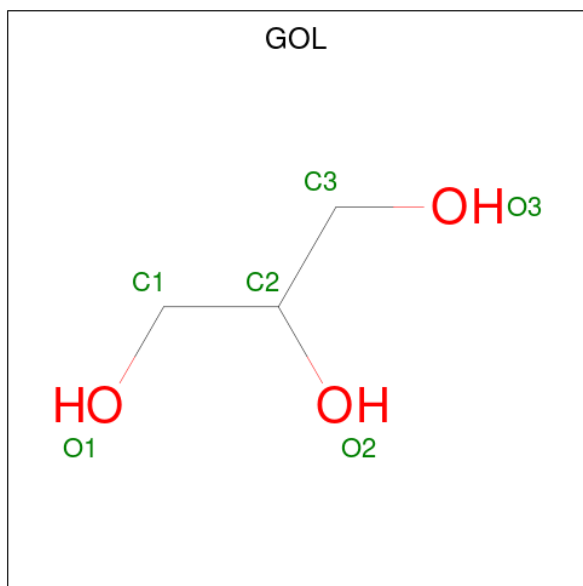
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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: C₃H₈O₃).



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

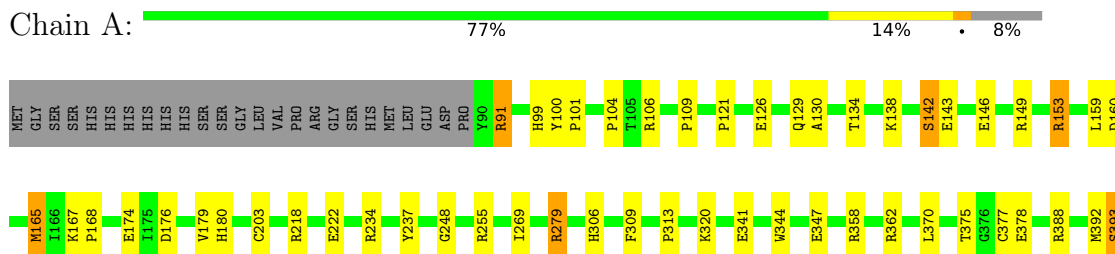
- Molecule 6 is water.

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, 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. 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. 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 1.10Å)	Xtriage
Refinement program	SHELX, SHELXL	Depositor
R, R_{free}	0.101 , 0.131 0.294 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.0	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.019 for h,-k,-l 0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2981	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CO, CL, GOL, K

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%)

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	392[A]	MET	Peptide
1	A	392[B]	MET	Peptide

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:OXT	1:A:393:SER:C	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
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%)	41 15

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%)	65 27

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

Sometimes 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 [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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.28	1 (20%)	5,5,5	1.36	1 (20%)
5	GOL	A	471	2	5,5,5	1.40	1 (20%)	5,5,5	1.96	2 (40%)
5	GOL	A	470[B]	-	5,5,5	0.51	0	5,5,5	2.02	3 (60%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	470[A]	GOL	O3-C3	2.36	1.52	1.42
5	A	471	GOL	C3-C2	2.14	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	471	GOL	O3-C3-C2	-2.99	95.85	110.20
5	A	470[B]	GOL	O1-C1-C2	-2.73	97.11	110.20
5	A	470[B]	GOL	C3-C2-C1	-2.39	102.41	111.70
5	A	471	GOL	C3-C2-C1	2.27	120.52	111.70
5	A	470[A]	GOL	O2-C2-C3	2.10	118.35	109.12
5	A	470[B]	GOL	O3-C3-C2	-2.02	100.54	110.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	470[B]	GOL	C1-C2-C3-O3
5	A	471	GOL	O1-C1-C2-C3
5	A	471	GOL	C1-C2-C3-O3
5	A	470[B]	GOL	O2-C2-C3-O3
5	A	471	GOL	O2-C2-C3-O3
5	A	471	GOL	O1-C1-C2-O2

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 [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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.