



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:52 AM UTC

PDB ID : 2B3H / pdb_00002b3h
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

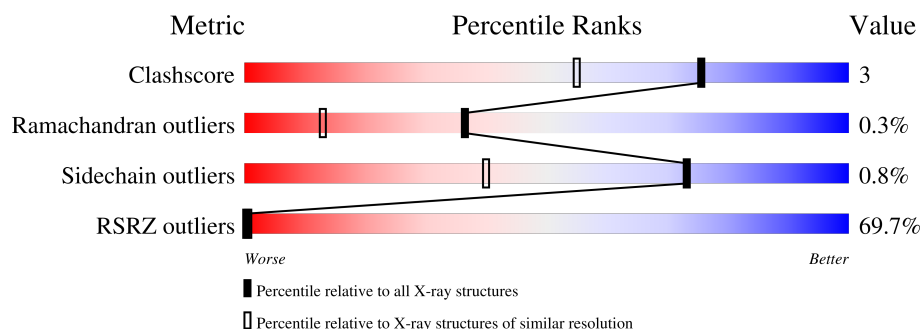
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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 $\leq 5\%$. 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	

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
1	A	304	Total	C	N	O	S	0	13	0
			2446	1540	438	445	23			

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 (CCD ID: CO) (formula: Co).

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

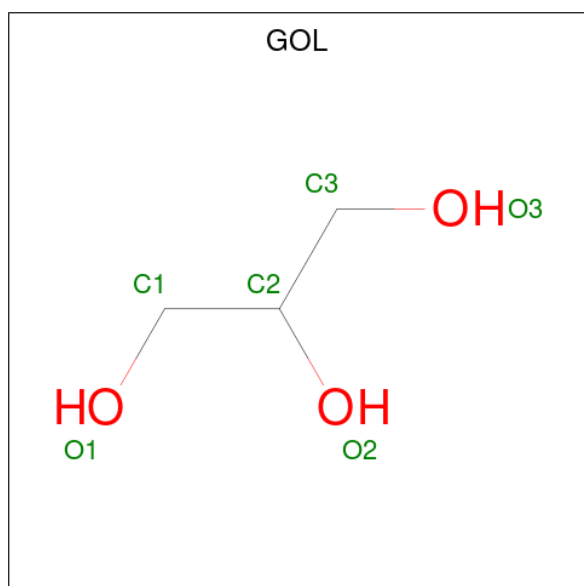
- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is GLYCEROL (CCD ID: 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

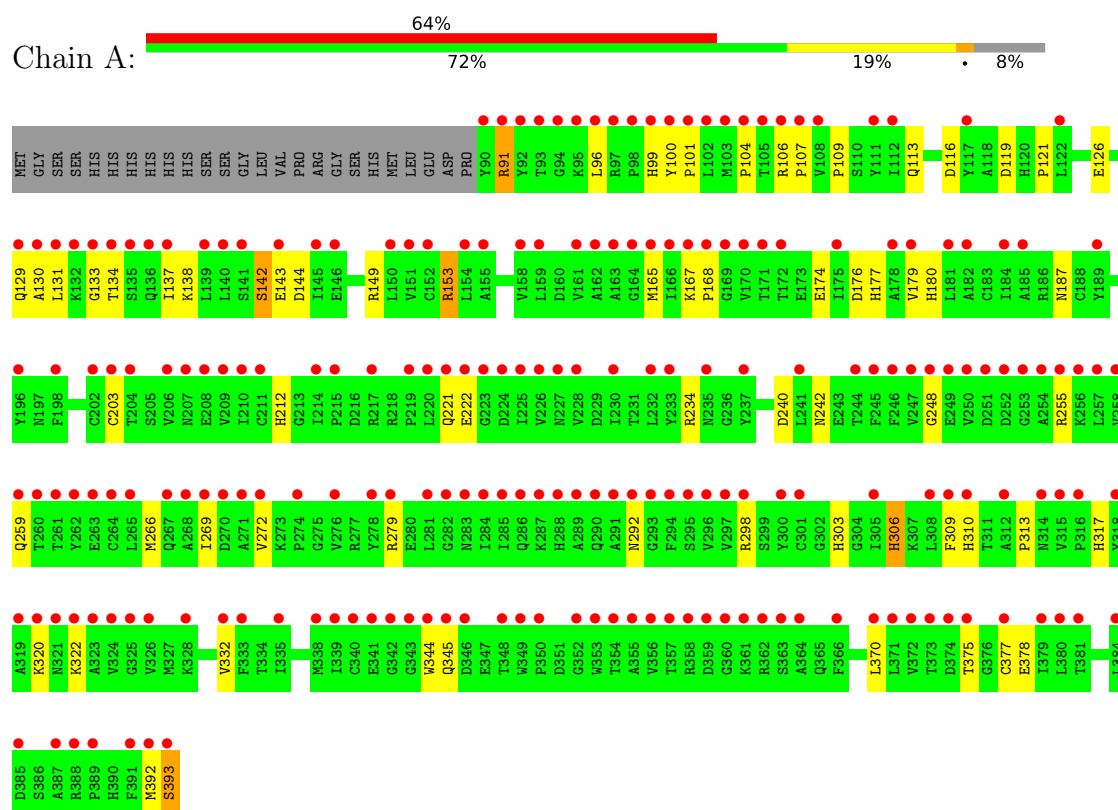
- Molecule 6 is water.

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 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, α , β , γ	47.29Å 77.30Å 48.34Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	20.00 – 1.10 20.00 – 1.10	Depositor EDS
% Data completeness (in resolution range)	91.6 (20.00-1.10) 89.7 (20.00-1.10)	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 0.293 , (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)	0.36 , 58.6	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, K, CO

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	1.67	18/2562 (0.7%)	1.73	60/3473 (1.7%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	SER	C-OXT	27.05	1.77	1.23
1	A	121	PRO	C-O	11.18	1.37	1.24
1	A	107	PRO	C-N	9.52	1.41	1.32
1	A	378	GLU	C-N	7.43	1.40	1.33
1	A	234	ARG	NE-CZ	-6.96	1.25	1.33
1	A	96	LEU	CB-CG	-6.75	1.40	1.53
1	A	306	HIS	ND1-CE1	-6.09	1.26	1.32
1	A	109	PRO	N-CD	-5.87	1.39	1.47
1	A	298	ARG	CD-NE	-5.85	1.38	1.46
1	A	137	ILE	C-O	5.81	1.30	1.24
1	A	332	VAL	C-N	5.76	1.40	1.33
1	A	104	PRO	N-CD	-5.60	1.40	1.47
1	A	168	PRO	N-CD	-5.36	1.40	1.47
1	A	142	SER	CA-CB	5.33	1.61	1.53
1	A	310	HIS	CA-C	5.29	1.58	1.52
1	A	317	HIS	ND1-CE1	5.28	1.37	1.32
1	A	298	ARG	CZ-NH2	-5.15	1.26	1.33
1	A	272	VAL	C-N	-5.01	1.27	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	CD-NE-CZ	15.48	146.08	124.40
1	A	143	GLU	CB-CG-CD	12.94	134.60	112.60
1	A	221	GLN	OE1-CD-NE2	-10.56	112.04	122.60
1	A	255	ARG	NE-CZ-NH2	10.53	128.68	119.20
1	A	104	PRO	CA-C-O	10.46	133.14	121.43
1	A	144	ASP	CA-CB-CG	10.39	122.99	112.60
1	A	375	THR	CA-CB-OG1	-9.85	94.83	109.60
1	A	121	PRO	O-C-N	-9.46	109.50	122.27
1	A	116	ASP	CA-CB-CG	8.99	121.59	112.60
1	A	104	PRO	O-C-N	-8.48	112.21	122.99
1	A	138	LYS	CG-CD-CE	8.41	130.65	111.30
1	A	91[A]	ARG	CB-CG-CD	8.27	130.32	111.30
1	A	91[B]	ARG	CB-CG-CD	8.27	130.32	111.30
1	A	344	TRP	CE3-CZ3-CH2	-8.02	110.67	121.10
1	A	259	GLN	OE1-CD-NE2	7.87	130.47	122.60
1	A	393	SER	CB-CA-C	7.77	124.86	110.10
1	A	119	ASP	CA-CB-CG	-7.74	104.86	112.60
1	A	104	PRO	N-CD-CG	7.73	114.79	103.20
1	A	165[A]	MET	CA-CB-CG	7.72	129.54	114.10
1	A	165[B]	MET	CA-CB-CG	7.72	129.54	114.10
1	A	313	PRO	N-CD-CG	7.51	112.81	103.80
1	A	168	PRO	O-C-N	-7.49	113.97	123.03
1	A	345	GLN	CG-CD-NE2	-7.42	105.26	116.40
1	A	153	ARG	NE-CZ-NH1	7.31	128.81	121.50
1	A	104	PRO	N-CA-CB	-7.26	97.22	103.32
1	A	377[A]	CYS	N-CA-CB	6.98	124.50	111.52
1	A	377[B]	CYS	N-CA-CB	6.98	124.50	111.52
1	A	393	SER	N-CA-C	-6.95	91.53	111.00
1	A	240	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	121	PRO	CA-C-N	6.50	133.06	122.65
1	A	121	PRO	C-N-CA	6.50	133.06	122.65
1	A	187	ASN	CA-CB-CG	-6.42	106.19	112.60
1	A	242	ASN	CA-CB-CG	6.35	118.95	112.60
1	A	393	SER	CA-C-O	-6.23	102.32	121.00
1	A	149	ARG	NE-CZ-NH2	-6.15	113.66	119.20
1	A	303	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
1	A	126	GLU	CG-CD-OE2	5.93	132.03	118.40
1	A	133	GLY	CA-C-O	5.90	127.26	119.58
1	A	106	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	A	104	PRO	CB-CG-CD	-5.85	87.37	106.10
1	A	306	HIS	CE1-NE2-CD2	-5.74	103.26	109.00
1	A	134	THR	CA-C-O	5.72	126.77	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	HIS	ND1-CE1-NE2	5.69	114.09	108.40
1	A	212	HIS	CE1-NE2-CD2	-5.60	103.40	109.00
1	A	174	GLU	CG-CD-OE1	5.58	131.24	118.40
1	A	142	SER	CA-CB-OG	-5.46	100.18	111.10
1	A	306	HIS	CB-CG-ND1	5.37	130.76	122.70
1	A	303	HIS	ND1-CE1-NE2	5.36	113.76	108.40
1	A	309	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	255	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	177	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	A	292	ASN	CA-C-O	5.30	125.85	119.59
1	A	222	GLU	CB-CG-CD	5.29	121.60	112.60
1	A	279[A]	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	A	279[B]	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	A	131	LEU	CA-C-N	-5.10	113.47	120.71
1	A	131	LEU	C-N-CA	-5.10	113.47	120.71
1	A	113	GLN	OE1-CD-NE2	5.09	127.69	122.60
1	A	168	PRO	CA-C-O	5.06	127.11	121.34
1	A	322	LYS	N-CA-CB	-5.01	103.57	111.39

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	14	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	7	0
All	All	2981	0	2427	15	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 (15) 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	1.25
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:266[B]:MET:HE2	6:A:574:HOH:O	1.84	0.76
1:A:99:HIS:HD2	6:A:952:HOH:O	1.91	0.53
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: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%)	36 13

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%)	271 (99%)	3 (1%)	65 29

All (3) 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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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[B]	-	5,5,5	0.54	0	5,5,5	2.17	3 (60%)
5	GOL	A	470[A]	-	5,5,5	1.30	1 (20%)	5,5,5	1.45	1 (20%)
5	GOL	A	471	2	5,5,5	1.48	1 (20%)	5,5,5	2.10	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[B]	-	-	2/4/4/4	-
5	GOL	A	470[A]	-	-	0/4/4/4	-
5	GOL	A	471	2	-	4/4/4/4	-

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	2.37	1.52	1.42
5	A	471	GOL	C3-C2	2.29	1.60	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	471	GOL	O3-C3-C2	-3.23	95.85	110.38
5	A	470[B]	GOL	O1-C1-C2	-2.95	97.11	110.38
5	A	470[B]	GOL	C3-C2-C1	-2.56	102.41	111.80
5	A	471	GOL	C3-C2-C1	2.38	120.52	111.80
5	A	470[A]	GOL	O2-C2-C3	2.22	118.35	109.18
5	A	470[B]	GOL	O3-C3-C2	-2.19	100.54	110.38
5	A	471	GOL	O1-C1-C2	-2.13	100.80	110.38

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

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, 95th 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 ²)	Q<0.9
1	A	304/329 (92%)	2.80	212 (69%) 0 0	7, 14, 30, 45	13 (4%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	VAL	7.3
1	A	291	ALA	7.2
1	A	294	PHE	7.1
1	A	246	PHE	6.7
1	A	293	GLY	6.6
1	A	96	LEU	5.9
1	A	349	TRP	5.9
1	A	247	VAL	5.7
1	A	92	TYR	5.5
1	A	257	LEU	5.4
1	A	166	ILE	5.4
1	A	225	ILE	5.3
1	A	223	GLY	5.2
1	A	91[A]	ARG	5.2
1	A	343	GLY	5.1
1	A	93	THR	5.1
1	A	340	CYS	5.1
1	A	344	TRP	5.1
1	A	375	THR	5.1
1	A	356	VAL	5.0
1	A	289	ALA	5.0
1	A	292	ASN	5.0
1	A	366	PHE	4.8
1	A	220	LEU	4.7
1	A	342	GLY	4.7
1	A	324	VAL	4.7
1	A	387	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	393	SER	4.6
1	A	252	ASP	4.6
1	A	389	PRO	4.6
1	A	90	TYR	4.6
1	A	139	LEU	4.5
1	A	134	THR	4.5
1	A	339	ILE	4.5
1	A	131	LEU	4.4
1	A	100	TYR	4.4
1	A	364	ALA	4.4
1	A	169	GLY	4.4
1	A	264	CYS	4.4
1	A	297	VAL	4.3
1	A	181	LEU	4.3
1	A	170[A]	VAL	4.3
1	A	254	ALA	4.3
1	A	353	TRP	4.3
1	A	108	VAL	4.2
1	A	357	THR	4.2
1	A	168	PRO	4.1
1	A	296	VAL	4.1
1	A	245	PHE	4.1
1	A	222	GLU	4.1
1	A	145	ILE	4.0
1	A	94	GLY	4.0
1	A	133	GLY	4.0
1	A	143	GLU	3.9
1	A	140	LEU	3.9
1	A	161	VAL	3.9
1	A	130	ALA	3.9
1	A	164	GLY	3.9
1	A	360	GLY	3.9
1	A	285	ILE	3.9
1	A	101	PRO	3.9
1	A	226	VAL	3.8
1	A	221	GLN	3.7
1	A	283	ASN	3.7
1	A	206	VAL	3.7
1	A	105[A]	THR	3.7
1	A	172	THR	3.7
1	A	261	THR	3.7
1	A	244	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	98	PRO	3.6
1	A	391	PHE	3.6
1	A	175	ILE	3.6
1	A	255	ARG	3.6
1	A	284	ILE	3.5
1	A	171	THR	3.5
1	A	326	VAL	3.5
1	A	102	LEU	3.5
1	A	319	ALA	3.5
1	A	207	ASN	3.4
1	A	332	VAL	3.4
1	A	219	PRO	3.4
1	A	301	CYS	3.4
1	A	355	ALA	3.4
1	A	211	CYS	3.3
1	A	374	ASP	3.3
1	A	269	ILE	3.3
1	A	373	THR	3.3
1	A	251	ASP	3.3
1	A	262	TYR	3.3
1	A	95	LYS	3.3
1	A	258	VAL	3.3
1	A	372	VAL	3.3
1	A	214	ILE	3.2
1	A	248	GLY	3.2
1	A	154	LEU	3.2
1	A	209	VAL	3.2
1	A	288	HIS	3.2
1	A	318	TYR	3.2
1	A	392[A]	MET	3.2
1	A	345	GLN	3.2
1	A	363	SER	3.2
1	A	350	PRO	3.2
1	A	370[A]	LEU	3.2
1	A	203	CYS	3.2
1	A	315	VAL	3.2
1	A	348	THR	3.2
1	A	210	ILE	3.2
1	A	359	ASP	3.1
1	A	265	LEU	3.1
1	A	260	THR	3.1
1	A	103	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	162	ALA	3.1
1	A	163	ALA	3.1
1	A	276	VAL	3.1
1	A	132	LYS	3.0
1	A	249	GLU	3.0
1	A	228	VAL	3.0
1	A	385	ASP	3.0
1	A	136	GLN	3.0
1	A	111	TYR	2.9
1	A	300	TYR	2.9
1	A	224	ASP	2.9
1	A	253	GLY	2.9
1	A	335	ILE	2.9
1	A	358	ARG	2.9
1	A	384	LEU	2.9
1	A	352	GLY	2.9
1	A	182	ALA	2.9
1	A	271	ALA	2.9
1	A	167	LYS	2.8
1	A	377[A]	CYS	2.8
1	A	215	PRO	2.8
1	A	259	GLN	2.8
1	A	322	LYS	2.8
1	A	268	ALA	2.8
1	A	295	SER	2.8
1	A	179[A]	VAL	2.8
1	A	282	GLY	2.8
1	A	137	ILE	2.8
1	A	104	PRO	2.8
1	A	380	LEU	2.8
1	A	290	GLN	2.7
1	A	202	CYS	2.7
1	A	320	LYS	2.7
1	A	155	ALA	2.7
1	A	321	ASN	2.7
1	A	122	LEU	2.7
1	A	159[A]	LEU	2.7
1	A	279[A]	ARG	2.7
1	A	381	THR	2.7
1	A	230	ILE	2.7
1	A	305	ILE	2.7
1	A	178	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	287	LYS	2.7
1	A	362	ARG	2.6
1	A	278	TYR	2.6
1	A	204	THR	2.6
1	A	232	LEU	2.6
1	A	152	CYS	2.6
1	A	346	ASP	2.6
1	A	361	LYS	2.6
1	A	281	LEU	2.6
1	A	99	HIS	2.6
1	A	158	VAL	2.6
1	A	323	ALA	2.6
1	A	341	GLU	2.6
1	A	196	TYR	2.6
1	A	309	PHE	2.5
1	A	272	VAL	2.5
1	A	314	ASN	2.5
1	A	298	ARG	2.5
1	A	165[A]	MET	2.5
1	A	333	PHE	2.5
1	A	107	PRO	2.5
1	A	354	THR	2.5
1	A	286	GLN	2.5
1	A	328	LYS	2.5
1	A	208	GLU	2.4
1	A	267	GLN	2.4
1	A	150	LEU	2.4
1	A	241	LEU	2.4
1	A	237	TYR	2.4
1	A	338	MET	2.4
1	A	227	ASN	2.4
1	A	184	ILE	2.4
1	A	388	ARG	2.4
1	A	141	SER	2.3
1	A	379	ILE	2.3
1	A	235	ASN	2.3
1	A	325	GLY	2.3
1	A	256	LYS	2.3
1	A	274	PRO	2.3
1	A	198	PHE	2.2
1	A	151	VAL	2.2
1	A	146	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	310	HIS	2.2
1	A	135	SER	2.2
1	A	263	GLU	2.2
1	A	117	TYR	2.2
1	A	106	ARG	2.1
1	A	312	ALA	2.1
1	A	308	LEU	2.1
1	A	233	TYR	2.1
1	A	185	ALA	2.1
1	A	371	LEU	2.1
1	A	316	PRO	2.1
1	A	270	ASP	2.0
1	A	112	ILE	2.0
1	A	97	ARG	2.0
1	A	189	TYR	2.0
1	A	217	ARG	2.0
1	A	129	GLN	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 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, 95th 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 ²)	Q<0.9
2	CO	A	404	1/1	0.73	0.20	16,16,16,16	1
3	K	A	405	1/1	0.79	0.17	11,11,11,11	0
5	GOL	A	470[A]	6/6	0.80	0.16	6,12,14,16	6
5	GOL	A	470[B]	6/6	0.80	0.16	10,12,13,13	6
5	GOL	A	471	6/6	0.81	0.17	20,27,37,38	0
4	CL	A	406	1/1	0.83	0.23	46,46,46,46	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CO	A	402	1/1	0.86	0.08	7,7,7,7	0
2	CO	A	401	1/1	0.88	0.08	8,8,8,8	0
2	CO	A	403	1/1	0.88	0.11	10,10,10,10	1

6.5 Other polymers [i](#)

There are no such residues in this entry.