



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:15 PM GMT

PDB ID : 3TFJ  
Title : DMSP-dependent demethylase from *P. ubique* - with cofactor THF  
Authors : Schuller, D.J.; Reisch, C.R.; Moran, M.A.; Whitman, W.B.; Lanzilotta, W.N.  
Deposited on : 2011-08-15  
Resolution : 1.60 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

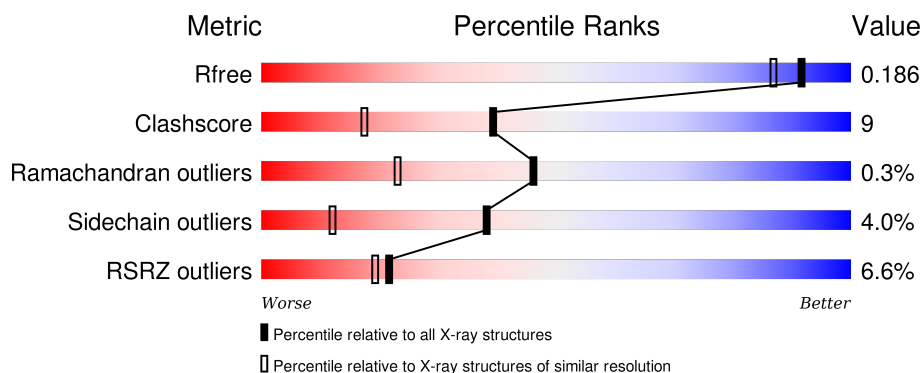
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	369	<div> <div>6%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	B	369	<div> <div>7%</div> <div>85%</div> <div>12%</div> <div>.</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
3	ACT	A	371[A]	-	-	-	X
3	ACT	B	371[A]	-	-	-	X
4	GOL	A	372	-	-	-	X
4	GOL	B	372	-	-	-	X

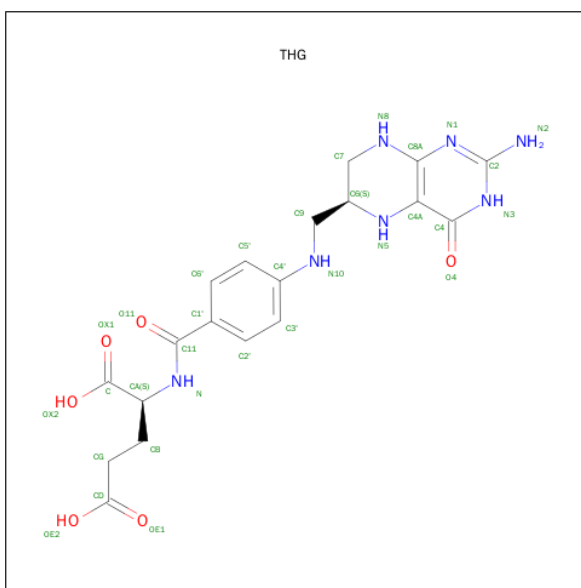


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GcvT-like Aminomethyltransferase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total 3107	C 2008	N 512	O 574	S 13	0	28	0
1	B	369	Total 3043	C 1955	N 502	O 572	S 14	0	16	0

- Molecule 2 is (6S)-5,6,7,8-TETRAHYDROFOLATE (three-letter code: THG) (formula:  $C_{19}H_{23}N_7O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 32	C 19	N 7	O 6	0	1
2	B	1	Total 32	C 19	N 7	O 6	0	1

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



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

- Molecule 4 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
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Na 1	0	0
5	A	1	Total 1	Na 1	0	0

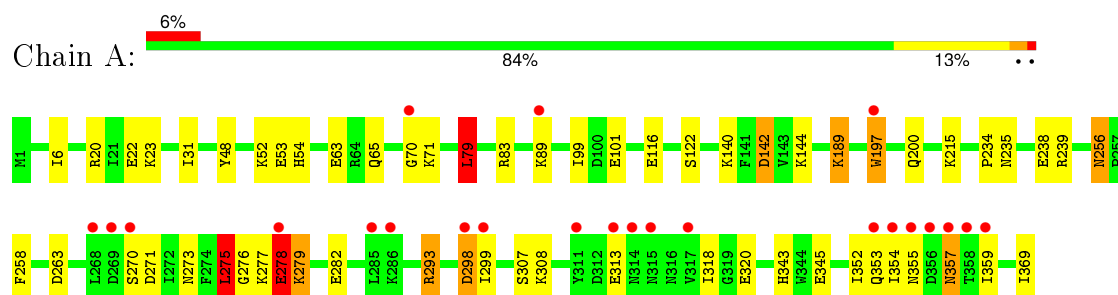
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	330	Total 330	O 330	0	1
6	B	403	Total 403	O 403	0	1

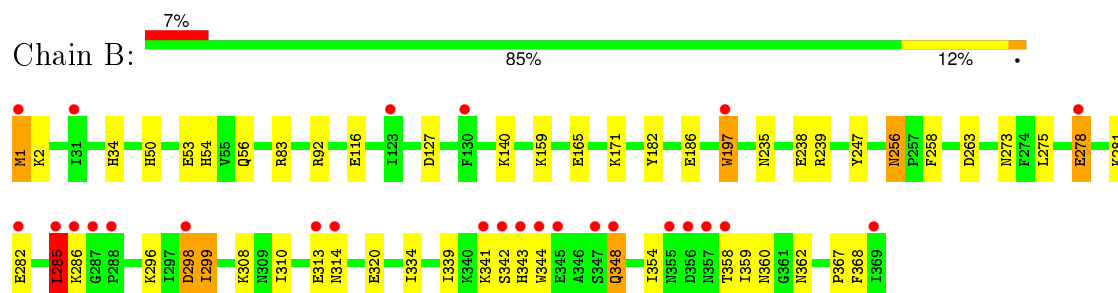
### 3 Residue-property plots

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: GcvT-like Aminomethyltransferase protein



- Molecule 1: GcvT-like Aminomethyltransferase protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.75Å 121.67Å 59.34Å 90.00° 100.30° 90.00°	Depositor
Resolution (Å)	36.11 – 1.60 36.11 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (36.11-1.60) 98.7 (36.11-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.35 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.126 , 0.176 0.138 , 0.186	Depositor DCC
$R_{free}$ test set	2389 reflections (2.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 97251 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6969	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 4.76% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: THG, GOL, ACT, NA

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	1.10	5/3254 (0.2%)	1.00	7/4371 (0.2%)
1	B	1.11	5/3151 (0.2%)	0.97	4/4239 (0.1%)
All	All	1.11	10/6405 (0.2%)	0.99	11/8610 (0.1%)

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
1	B	0	2
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	320	GLU	CB-CG	-7.70	1.37	1.52
1	B	83	ARG	CG-CD	-7.44	1.33	1.51
1	B	278[A]	GLU	CB-CG	6.14	1.63	1.52
1	B	278[B]	GLU	CB-CG	6.14	1.63	1.52
1	A	282	GLU	CG-CD	5.67	1.60	1.51
1	A	70	GLY	N-CA	5.41	1.54	1.46
1	A	279	LYS	N-CA	-5.41	1.35	1.46
1	B	182	TYR	CD1-CE1	5.37	1.47	1.39
1	A	83	ARG	CG-CD	-5.20	1.39	1.51
1	A	101	GLU	CB-CG	5.10	1.61	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278[A]	GLU	CA-CB-CG	7.89	130.77	113.40
1	A	278[B]	GLU	CA-CB-CG	7.89	130.77	113.40
1	B	92	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	293	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	285	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	20	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	142	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	275	LEU	CB-CG-CD1	5.51	120.38	111.00
1	B	92	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	275	LEU	CB-CG-CD2	5.06	119.61	111.00
1	A	79	LEU	CB-CG-CD2	5.01	119.52	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	LYS	Peptide
1	B	1[A]	MET	Peptide
1	B	1[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	3107	0	3186	72	0
1	B	3043	0	3054	43	0
2	A	32	0	21	4	0
2	B	32	0	21	1	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	6	0	8	0	0
4	B	6	0	8	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	330	0	0	15	0
6	B	403	0	0	11	0
All	All	6969	0	6304	112	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 9.

All (112) 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:B:367:PRO:HB2	6:B:715:HOH:O	1.46	1.13
1:A:299:ILE:HG23	1:A:359[A]:ILE:CD1	1.95	0.95
1:A:99:ILE:HD11	1:A:275:LEU:O	1.68	0.93
1:A:23[B]:LYS:HE2	1:B:1[B]:MET:CE	2.02	0.90
1:B:282:GLU:O	1:B:285:LEU:HD12	1.77	0.84
1:A:369:ILE:HD12	1:A:369:ILE:O	1.78	0.82
1:B:116[A]:GLU:HG2	6:B:542:HOH:O	1.81	0.81
1:A:99:ILE:C	1:A:99:ILE:HD12	2.01	0.81
1:A:63:GLU:HG2	1:A:197[B]:TRP:CZ2	2.17	0.79
1:A:299:ILE:HG23	1:A:359[A]:ILE:HD12	1.66	0.75
1:A:299:ILE:CG2	1:A:359[A]:ILE:CD1	2.65	0.74
1:B:354:ILE:HD12	1:B:359:ILE:HD12	1.69	0.74
1:A:369:ILE:HD12	1:A:369:ILE:C	2.08	0.74
1:A:23[B]:LYS:CE	1:B:1[B]:MET:HE3	2.18	0.73
1:B:273[B]:ASN:ND2	6:B:586:HOH:O	2.21	0.73
1:A:53[B]:GLU:HG3	6:A:680:HOH:O	1.89	0.72
1:A:369:ILE:HD11	6:A:460:HOH:O	1.89	0.72
1:B:235:ASN:HD22	1:B:238:GLU:H	1.37	0.71
1:A:23[B]:LYS:HE2	1:B:1[B]:MET:HE3	1.70	0.71
1:B:50:HIS:HD2	1:B:56:GLN:HE21	1.38	0.71
2:B:370[A]:THG:OE1	6:B:671:HOH:O	2.08	0.71
1:A:235:ASN:HD22	1:A:238:GLU:H	1.40	0.69
1:A:23[B]:LYS:CE	1:B:1[B]:MET:CE	2.71	0.67
1:A:23[A]:LYS:NZ	6:A:419:HOH:O	2.23	0.67
1:A:48:TYR:CZ	1:A:52[B]:LYS:HD2	2.30	0.66
1:A:299:ILE:HG23	1:A:359[A]:ILE:HD11	1.75	0.66
1:A:63:GLU:HG2	1:A:197[B]:TRP:CH2	2.31	0.66
1:A:345:GLU:CD	1:A:345:GLU:H	2.01	0.63
1:A:307:SER:HB3	1:A:320:GLU:CG	2.29	0.63
1:B:50:HIS:CD2	1:B:56:GLN:HE21	2.17	0.62
1:B:299:ILE:HG12	1:B:359:ILE:HD13	1.82	0.61
1:B:298[B]:ASP:OD1	1:B:360:ASN:O	2.19	0.60
1:A:299:ILE:HG12	1:A:359[A]:ILE:HD13	1.84	0.60
1:A:189:LYS:HE3	6:A:659:HOH:O	2.02	0.59
1:B:54:HIS:HD2	1:B:159:LYS:NZ	2.02	0.58
1:A:308[A]:LYS:HE2	1:A:353:GLN:O	2.04	0.58
1:B:247:TYR:OH	4:B:372:GOL:H31	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:CD1	1:A:369:ILE:C	2.71	0.58
1:A:63:GLU:CG	1:A:197[B]:TRP:CH2	2.87	0.57
1:A:116[A]:GLU:OE2	6:A:663:HOH:O	2.17	0.57
1:A:357:ASN:HD22	1:A:359[B]:ILE:HD11	1.70	0.57
1:A:307:SER:HB3	1:A:320:GLU:HG3	1.87	0.57
1:A:63:GLU:OE2	1:A:197[B]:TRP:CE2	2.59	0.56
1:A:99:ILE:CD1	1:A:275:LEU:O	2.50	0.56
1:A:89[B]:LYS:HE2	6:A:676:HOH:O	2.06	0.56
1:A:299:ILE:CG2	1:A:359[A]:ILE:HD12	2.34	0.55
1:A:140[B]:LYS:HE3	1:A:140[B]:LYS:HA	1.87	0.55
1:B:354:ILE:HD12	1:B:359:ILE:CD1	2.36	0.54
1:B:310:ILE:HD11	1:B:339:ILE:CD1	2.37	0.54
1:B:186:GLU:OE1	6:B:693:HOH:O	2.18	0.54
1:A:369:ILE:CD1	6:A:461:HOH:O	2.56	0.54
2:A:370[A]:THG:C	6:A:737:HOH:O	2.55	0.54
1:A:318:ILE:HD12	1:A:343:HIS:CG	2.44	0.53
1:A:23[B]:LYS:HE2	1:B:1[B]:MET:HE1	1.88	0.53
1:A:369:ILE:HD12	6:A:461:HOH:O	2.09	0.52
1:A:63:GLU:CG	1:A:197[B]:TRP:CZ2	2.90	0.51
2:A:370[A]:THG:OE1	6:A:670:HOH:O	2.19	0.51
1:B:247:TYR:OH	4:B:372:GOL:C3	2.58	0.50
1:A:256:ASN:HD22	1:A:258:PHE:H	1.58	0.50
1:B:197[A]:TRP:CH2	1:B:239:ARG:HD3	2.46	0.50
1:A:197[A]:TRP:HE3	1:A:234:PRO:HB3	1.77	0.49
1:A:22:GLU:O	1:B:1[B]:MET:HE2	2.13	0.49
1:B:368:PHE:N	6:B:715:HOH:O	2.44	0.49
1:A:6:ILE:HD11	1:A:31:ILE:HD11	1.95	0.48
1:A:48:TYR:CE2	1:A:52[B]:LYS:HD2	2.48	0.48
1:A:278[A]:GLU:OE1	1:A:279:LYS:HD2	2.14	0.48
1:A:308[B]:LYS:HE2	1:A:308[B]:LYS:HB2	1.44	0.48
1:A:63:GLU:OE2	1:A:197[B]:TRP:CD2	2.67	0.47
1:B:165:GLU:OE1	6:B:692:HOH:O	2.20	0.47
1:B:341:LYS:HA	1:B:344:TRP:CE2	2.49	0.47
1:B:343:HIS:CD2	1:B:348:GLN:HE22	2.33	0.47
1:A:23[B]:LYS:CD	1:B:1[B]:MET:HE1	2.44	0.47
2:A:370[A]:THG:HCA	6:A:737:HOH:O	2.14	0.47
2:A:370[A]:THG:CA	6:A:737:HOH:O	2.62	0.46
1:B:342:SER:HG	1:B:343:HIS:CE1	2.30	0.46
1:A:53[A]:GLU:HG3	1:A:54:HIS:CD2	2.51	0.46
1:A:200:GLN:NE2	6:A:652:HOH:O	2.49	0.45
1:A:276:GLY:C	1:A:278[A]:GLU:HB2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ILE:CG1	1:A:359[A]:ILE:HD13	2.46	0.45
1:B:310:ILE:HD11	1:B:339:ILE:HD13	1.98	0.45
1:B:313:GLU:CD	1:B:313:GLU:H	2.20	0.45
1:A:197[A]:TRP:CH2	1:A:239:ARG:HD3	2.52	0.45
1:B:278[B]:GLU:HG2	6:B:467:HOH:O	2.16	0.45
1:B:343:HIS:CD2	1:B:348:GLN:NE2	2.85	0.44
1:B:140[B]:LYS:HB3	1:B:140[B]:LYS:HE3	1.82	0.44
1:A:53[A]:GLU:HG3	1:A:54:HIS:NE2	2.32	0.44
1:A:354:ILE:HG12	1:A:359[A]:ILE:HG21	2.00	0.43
1:A:79:LEU:HD22	1:A:275:LEU:HD13	2.00	0.43
1:A:65:GLN:HE22	1:A:122[A]:SER:HB2	1.80	0.43
1:A:23[B]:LYS:CD	1:B:1[B]:MET:CE	2.96	0.43
1:B:53[A]:GLU:HG3	6:B:531:HOH:O	2.18	0.43
1:A:357:ASN:ND2	1:A:359[B]:ILE:HD11	2.33	0.43
1:A:278[A]:GLU:HB3	1:A:279:LYS:HG3	2.01	0.43
1:B:296:LYS:HG2	1:B:334:ILE:HG22	2.01	0.43
1:A:71[A]:LYS:HE3	1:A:142:ASP:OD1	2.19	0.42
1:A:278[B]:GLU:CA	1:A:278[B]:GLU:OE1	2.61	0.42
1:A:293:ARG:HD2	6:A:536:HOH:O	2.19	0.42
1:A:354:ILE:HG12	1:A:359[A]:ILE:CG2	2.49	0.42
1:A:215[A]:LYS:HG3	6:A:585:HOH:O	2.19	0.41
1:A:276:GLY:HA2	1:A:278[A]:GLU:OE1	2.21	0.41
1:B:299:ILE:CG1	1:B:359:ILE:HD13	2.49	0.41
1:B:34:HIS:HE1	1:B:127:ASP:OD2	2.03	0.41
1:B:278[B]:GLU:HA	1:B:281:LYS:HE2	2.02	0.41
1:B:171[A]:LYS:HE3	6:B:661:HOH:O	2.20	0.41
1:A:53[A]:GLU:CG	1:A:54:HIS:CD2	3.03	0.41
1:A:352:ILE:CG2	1:A:359[A]:ILE:HG23	2.51	0.40
1:B:1[A]:MET:CE	6:B:452:HOH:O	2.70	0.40
1:B:256:ASN:HD22	1:B:258:PHE:H	1.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	395/369 (107%)	383 (97%)	9 (2%)	3 (1%)	24	6
1	B	382/369 (104%)	370 (97%)	12 (3%)	0	100	100
All	All	777/738 (105%)	753 (97%)	21 (3%)	3 (0%)	46	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278[A]	GLU
1	A	278[B]	GLU
1	A	355	ASN

### 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	352/324 (109%)	334 (95%)	18 (5%)	29	7
1	B	340/324 (105%)	325 (96%)	15 (4%)	35	10
All	All	692/648 (107%)	659 (95%)	33 (5%)	38	8

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	144[A]	LYS
1	A	144[B]	LYS
1	A	189	LYS
1	A	197[A]	TRP
1	A	197[B]	TRP
1	A	256	ASN
1	A	263	ASP
1	A	270	SER
1	A	271[A]	ASP

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Mol	Chain	Res	Type
1	A	271[B]	ASP
1	A	273[A]	ASN
1	A	273[B]	ASN
1	A	275	LEU
1	A	298[A]	ASP
1	A	298[B]	ASP
1	A	313	GLU
1	A	357	ASN
1	B	2	LYS
1	B	197[A]	TRP
1	B	197[B]	TRP
1	B	256	ASN
1	B	263	ASP
1	B	285	LEU
1	B	286	LYS
1	B	298[A]	ASP
1	B	298[B]	ASP
1	B	299	ILE
1	B	308	LYS
1	B	314	ASN
1	B	348	GLN
1	B	358	THR
1	B	362	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	200	GLN
1	A	235	ASN
1	A	256	ASN
1	A	316	ASN
1	A	357	ASN
1	B	24	GLN
1	B	34	HIS
1	B	50	HIS
1	B	54	HIS
1	B	211	GLN
1	B	228	ASN
1	B	235	ASN
1	B	256	ASN
1	B	314	ASN

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Mol	Chain	Res	Type
1	B	316	ASN
1	B	348	GLN
1	B	353	GLN
1	B	360	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z  > 2$
2	THG	A	370[A]	-	26,34,34	1.05	3 (11%)	28,47,47	1.88	7 (25%)
3	ACT	A	371[A]	-	1,3,3	2.12	1 (100%)	0,3,3	0.00	-
4	GOL	A	372	-	5,5,5	0.64	0	5,5,5	0.98	0
2	THG	B	370[A]	-	26,34,34	1.24	3 (11%)	28,47,47	1.50	6 (21%)
3	ACT	B	371[A]	-	1,3,3	2.65	1 (100%)	0,3,3	0.00	-
4	GOL	B	372	-	5,5,5	0.78	0	5,5,5	1.37	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
2	THG	A	370[A]	-	-	0/16/31/31	0/3/3/3
3	ACT	A	371[A]	-	-	0/0/0/0	0/0/0/0
4	GOL	A	372	-	-	0/4/4/4	0/0/0/0
2	THG	B	370[A]	-	-	0/16/31/31	0/3/3/3
3	ACT	B	371[A]	-	-	0/0/0/0	0/0/0/0
4	GOL	B	372	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	370[A]	THG	C4A-C8A	2.05	1.45	1.41
3	A	371[A]	ACT	CH3-C	2.12	1.51	1.48
2	A	370[A]	THG	C7-N8	2.30	1.49	1.46
2	B	370[A]	THG	C4-N3	2.49	1.37	1.33
2	B	370[A]	THG	C4A-C8A	2.55	1.46	1.41
3	B	371[A]	ACT	CH3-C	2.65	1.52	1.48
2	A	370[A]	THG	C4-N3	2.98	1.38	1.33
2	B	370[A]	THG	C7-N8	3.84	1.51	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370[A]	THG	C3'-C2'-C1'	-2.78	117.54	120.76
2	A	370[A]	THG	C1'-C11-N	-2.73	112.06	116.93
2	A	370[A]	THG	C3'-C4'-N10	-2.15	116.94	121.06
2	B	370[A]	THG	O11-C11-C1'	-2.10	117.38	120.97
2	B	370[A]	THG	C3'-C2'-C1'	-2.01	118.43	120.76
2	A	370[A]	THG	C4A-C8A-N8	2.31	121.15	118.43
2	B	370[A]	THG	C8A-C4A-N5	2.32	121.77	118.85
2	A	370[A]	THG	C6'-C1'-C2'	2.73	122.66	118.60
2	B	370[A]	THG	O11-C11-N	2.85	127.58	122.44
2	B	370[A]	THG	C4-N3-C2	3.21	120.40	115.94
2	B	370[A]	THG	C2-N1-C8A	3.35	122.06	114.54
2	A	370[A]	THG	O11-C11-N	4.32	130.24	122.44
2	A	370[A]	THG	C2-N1-C8A	4.73	125.18	114.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	370[A]	THG	4	0
2	B	370[A]	THG	1	0
4	B	372	GOL	2	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, 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	369/369 (100%)	0.13	23 (6%)	24 21	14, 26, 44, 62	0
1	B	369/369 (100%)	0.07	26 (7%)	19 17	13, 25, 45, 56	0
All	All	738/738 (100%)	0.10	49 (6%)	22 19	13, 25, 45, 62	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	LEU	7.4
1	A	355	ASN	6.0
1	B	369	ILE	4.9
1	A	314	ASN	4.6
1	B	286	LYS	4.5
1	A	356	ASP	4.5
1	A	285	LEU	4.4
1	A	313	GLU	4.4
1	B	1[A]	MET	4.2
1	A	357	ASN	4.2
1	B	287	GLY	4.0
1	A	354	ILE	3.8
1	B	342	SER	3.8
1	B	344	TRP	3.7
1	A	359[A]	ILE	3.6
1	A	270	SER	3.5
1	A	269	ASP	3.5
1	A	197[A]	TRP	3.4
1	B	314	ASN	3.4
1	A	358	THR	3.4
1	A	286[A]	LYS	3.3
1	B	357	ASN	3.2
1	A	298[A]	ASP	3.2
1	B	197[A]	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	353	GLN	3.1
1	A	70	GLY	3.0
1	B	278[A]	GLU	2.9
1	B	348	GLN	2.7
1	B	298[A]	ASP	2.7
1	B	358	THR	2.7
1	A	317	VAL	2.6
1	A	311	TYR	2.6
1	B	343	HIS	2.6
1	B	341	LYS	2.5
1	A	268	LEU	2.5
1	B	282	GLU	2.5
1	B	31	ILE	2.5
1	B	288	PRO	2.4
1	B	345	GLU	2.3
1	B	123	ILE	2.3
1	A	89[A]	LYS	2.3
1	B	347	SER	2.3
1	B	355	ASN	2.2
1	A	299	ILE	2.2
1	B	130	PHE	2.1
1	A	278[A]	GLU	2.1
1	A	315	ASN	2.1
1	B	313	GLU	2.1
1	B	356	ASP	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
4	GOL	A	372	6/6	0.87	0.30	6.96	37,52,55,57	0
3	ACT	B	371[A]	4/4	0.89	0.34	5.83	33,36,36,36	4
3	ACT	A	371[A]	4/4	0.56	0.33	4.70	41,42,42,42	4
4	GOL	B	372	6/6	0.81	0.21	4.20	39,54,60,60	0
2	THG	A	370[A]	32/32	0.73	0.16	1.34	29,39,49,51	32
5	NA	B	373	1/1	1.00	0.14	1.26	21,21,21,21	0
2	THG	B	370[A]	32/32	0.78	0.17	1.21	26,37,47,49	32
5	NA	A	373	1/1	0.99	0.09	-0.41	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.