



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:49 am GMT

PDB ID : 1NMU  
Title : MBP-L30  
Authors : Chao, J.A.; Prasad, G.S.; White, S.A.; Stout, C.D.; Williamson, J.R.  
Deposited on : 2003-01-10  
Resolution : 2.31 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

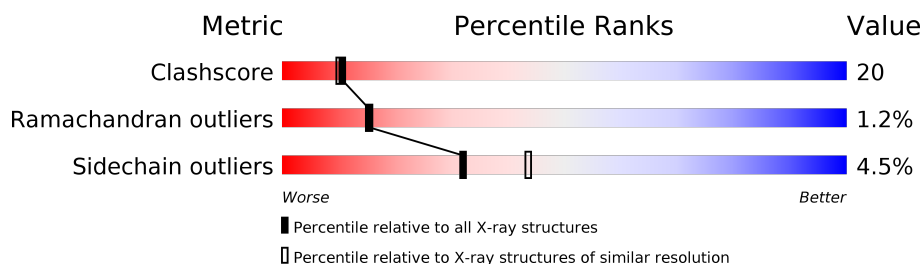
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	382	
1	C	382	
2	B	104	
2	D	104	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7593 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 maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2843	1828	463	546	6			
1	C	368	Total	C	N	O	S	0	0	0
			2843	1828	463	546	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING MET	UNP P02928
A	367	ASN	-	CLONING ARTIFACT	UNP P02928
A	368	SER	-	CLONING ARTIFACT	UNP P02928
A	369	SER	-	CLONING ARTIFACT	UNP P02928
A	370	SER	-	CLONING ARTIFACT	UNP P02928
A	371	VAL	-	CLONING ARTIFACT	UNP P02928
A	372	PRO	-	CLONING ARTIFACT	UNP P02928
A	373	GLY	-	CLONING ARTIFACT	UNP P02928
A	374	ARG	-	CLONING ARTIFACT	UNP P02928
A	375	GLY	-	CLONING ARTIFACT	UNP P02928
A	376	SER	-	CLONING ARTIFACT	UNP P02928
A	377	ILE	-	CLONING ARTIFACT	UNP P02928
A	378	GLU	-	CLONING ARTIFACT	UNP P02928
A	379	GLY	-	CLONING ARTIFACT	UNP P02928
A	380	ARG	-	CLONING ARTIFACT	UNP P02928
A	381	ALA	-	CLONING ARTIFACT	UNP P02928
C	0	MET	-	INITIATING MET	UNP P02928
C	367	ASN	-	CLONING ARTIFACT	UNP P02928
C	368	SER	-	CLONING ARTIFACT	UNP P02928
C	369	SER	-	CLONING ARTIFACT	UNP P02928
C	370	SER	-	CLONING ARTIFACT	UNP P02928
C	371	VAL	-	CLONING ARTIFACT	UNP P02928
C	372	PRO	-	CLONING ARTIFACT	UNP P02928
C	373	GLY	-	CLONING ARTIFACT	UNP P02928
C	374	ARG	-	CLONING ARTIFACT	UNP P02928

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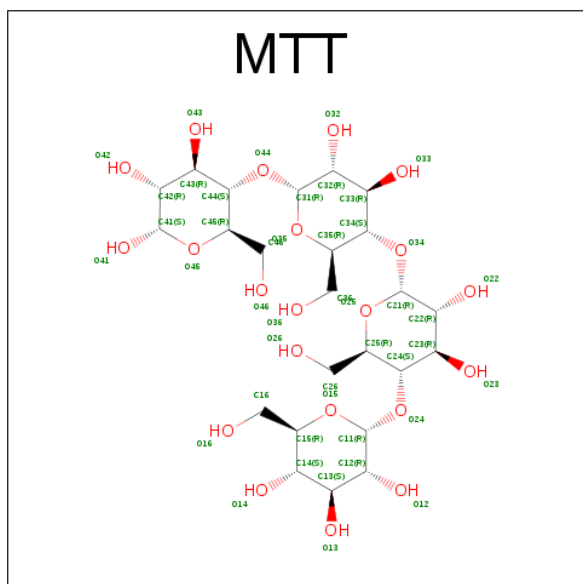
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Chain	Residue	Modelled	Actual	Comment	Reference
C	375	GLY	-	CLONING ARTIFACT	UNP P02928
C	376	SER	-	CLONING ARTIFACT	UNP P02928
C	377	ILE	-	CLONING ARTIFACT	UNP P02928
C	378	GLU	-	CLONING ARTIFACT	UNP P02928
C	379	GLY	-	CLONING ARTIFACT	UNP P02928
C	380	ARG	-	CLONING ARTIFACT	UNP P02928
C	381	ALA	-	CLONING ARTIFACT	UNP P02928

- Molecule 2 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			795	511	133	150	1			
2	D	103	Total	C	N	O	S	0	0	0
			790	508	132	149	1			

- Molecule 3 is MALTOTETRAOSE (three-letter code: MTT) (formula:  $C_{24}H_{42}O_{21}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			45	24	21		
3	C	1	Total	C	O	0	0
			45	24	21		

- Molecule 4 is water.

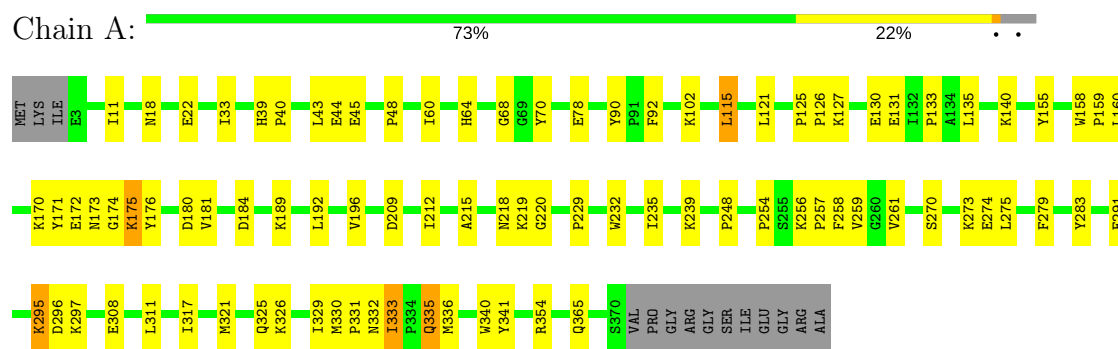
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total 130	O 130	0	0
4	B	26	Total 26	O 26	0	0
4	C	75	Total 75	O 75	0	0
4	D	1	Total 1	O 1	0	0

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

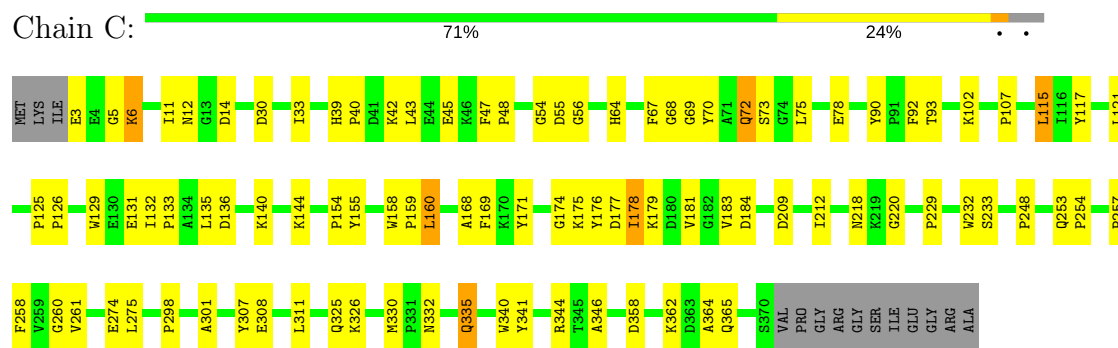
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

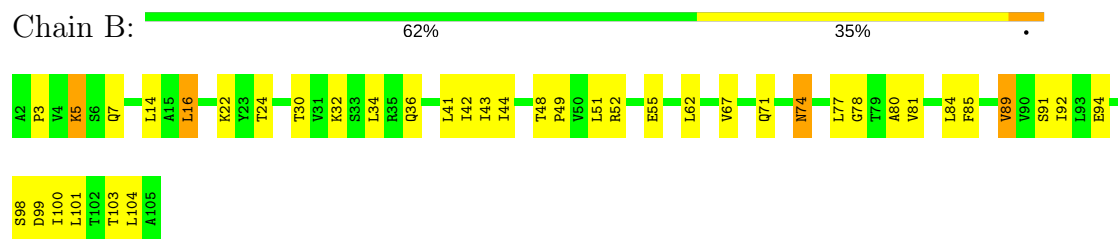
- Molecule 1: maltose-binding periplasmic protein



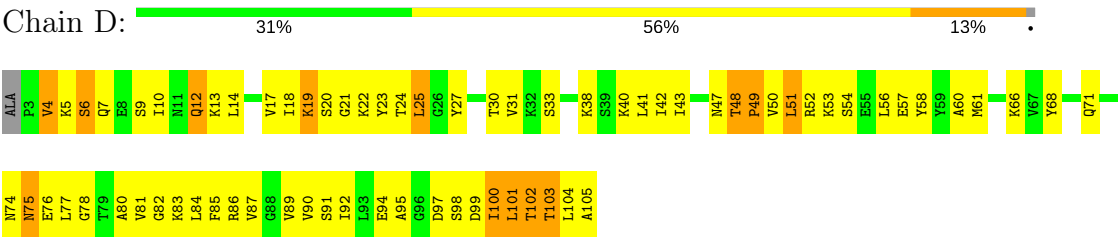
- Molecule 1: maltose-binding periplasmic protein



- Molecule 2: 60S ribosomal protein L30



- Molecule 2: 60S ribosomal protein L30



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.65Å 118.39Å 153.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.31	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-2.31)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP



## 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: MTT

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	0.36	0/2912	0.59	0/3955
1	C	0.34	0/2912	0.57	0/3955
2	B	0.36	0/804	0.66	0/1080
2	D	0.31	0/799	0.54	0/1072
All	All	0.35	0/7427	0.59	0/10062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2843	0	2801	78	0
1	C	2843	0	2801	91	0
2	B	795	0	850	36	0
2	D	790	0	846	105	0
3	A	45	0	39	7	0
3	C	45	0	41	7	0
4	A	130	0	0	4	0
4	B	26	0	0	0	0
4	C	75	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	7593	0	7378	302	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 20.

All (302) 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:155:TYR:HB2	3:A:382:MTT:H262	1.28	1.14
2:D:20:SER:HB2	2:D:97:ASP:H	1.20	1.06
1:C:335:GLN:NE2	1:C:335:GLN:H	1.60	0.99
1:A:64:HIS:HD2	1:A:261:VAL:H	1.12	0.97
1:C:155:TYR:HB2	3:C:382:MTT:H262	1.47	0.96
1:C:335:GLN:HE21	1:C:335:GLN:H	1.16	0.92
1:A:335:GLN:NE2	1:A:335:GLN:H	1.68	0.91
2:D:101:LEU:HD22	2:D:101:LEU:H	1.35	0.91
2:B:22:LYS:HD2	2:B:94:GLU:HG3	1.53	0.91
1:A:181:VAL:HB	1:A:365:GLN:HE22	1.40	0.86
1:A:90:TYR:HE1	1:A:308:GLU:HG2	1.40	0.86
2:D:5:LYS:HB2	2:D:71:GLN:HE21	1.41	0.85
1:C:209:ASP:OD1	1:C:212:ILE:HG12	1.78	0.83
2:D:20:SER:HB2	2:D:97:ASP:N	1.93	0.82
2:D:75:ASN:HD22	2:D:76:GLU:H	1.29	0.81
1:C:68:GLY:HA3	1:C:332:ASN:O	1.81	0.81
1:A:155:TYR:CB	3:A:382:MTT:H262	2.11	0.80
2:D:33:SER:HA	2:D:38:LYS:HE2	1.63	0.80
2:D:13:LYS:HG3	2:D:100:ILE:HG22	1.63	0.79
1:C:64:HIS:HD2	1:C:261:VAL:H	1.29	0.79
2:D:104:LEU:H	2:D:104:LEU:HD12	1.48	0.78
2:D:95:ALA:HB3	2:D:101:LEU:HD21	1.65	0.78
1:A:335:GLN:HE21	1:A:335:GLN:H	1.29	0.78
2:D:102:THR:HG22	2:D:103:THR:H	1.49	0.76
1:C:48:PRO:HG3	1:C:70:TYR:CE1	2.20	0.76
1:A:181:VAL:HB	1:A:365:GLN:NE2	2.00	0.76
1:A:155:TYR:HB2	3:A:382:MTT:C26	2.13	0.76
1:A:90:TYR:CE1	1:A:308:GLU:HG2	2.21	0.75
1:C:33:ILE:HD13	1:C:275:LEU:HD13	1.67	0.75
2:B:103:THR:HG23	2:B:104:LEU:HD13	1.68	0.74
1:A:175:LYS:HA	1:A:175:LYS:HE2	1.68	0.74
1:C:184:ASP:HB2	1:C:365:GLN:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:LEU:HD23	2:D:42:ILE:N	2.03	0.74
2:D:41:LEU:HD23	2:D:42:ILE:H	1.54	0.72
2:D:74:ASN:ND2	2:D:86:ARG:HD3	2.05	0.71
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.72	0.71
1:C:181:VAL:HB	1:C:365:GLN:HE22	1.57	0.70
2:D:74:ASN:HD22	2:D:86:ARG:HB3	1.56	0.69
2:B:48:THR:HG23	2:B:51:LEU:HB2	1.75	0.69
2:D:75:ASN:ND2	2:D:76:GLU:H	1.90	0.69
1:C:181:VAL:HB	1:C:365:GLN:NE2	2.08	0.68
2:D:95:ALA:CB	2:D:101:LEU:HD21	2.23	0.68
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.29	0.67
2:D:6:SER:O	2:D:7:GLN:HG3	1.93	0.67
2:D:51:LEU:HA	2:D:54:SER:OG	1.94	0.67
2:D:9:SER:O	2:D:12:GLN:HG3	1.96	0.66
2:D:54:SER:HA	2:D:57:GLU:OE2	1.94	0.66
2:B:32:LYS:HE2	2:B:36:GLN:HE22	1.59	0.66
2:B:41:LEU:HD12	2:B:92:ILE:HD13	1.78	0.66
1:C:178:ILE:HD13	1:C:178:ILE:H	1.60	0.65
1:C:42:LYS:HE2	3:C:382:MTT:O42	1.96	0.65
2:D:43:ILE:HB	2:D:90:VAL:CG1	2.26	0.65
2:D:24:THR:HG23	2:D:91:SER:HB3	1.77	0.65
1:A:43:LEU:CD1	1:A:60:ILE:HD11	2.26	0.65
2:B:7:GLN:NE2	2:B:77:LEU:HD23	2.11	0.65
1:C:3:GLU:CB	1:C:6:LYS:HE3	2.26	0.64
2:D:77:LEU:O	2:D:81:VAL:HG23	1.97	0.64
2:D:99:ASP:OD2	2:D:104:LEU:HD21	1.98	0.64
1:C:178:ILE:HD13	1:C:178:ILE:N	2.13	0.64
1:C:48:PRO:HG3	1:C:70:TYR:HE1	1.63	0.64
1:A:335:GLN:NE2	1:A:335:GLN:N	2.45	0.63
1:A:45:GLU:O	1:A:48:PRO:HD2	1.98	0.63
1:A:209:ASP:OD1	1:A:212:ILE:HG12	1.97	0.63
2:D:83:LYS:HG2	2:D:85:PHE:CZ	2.34	0.63
1:A:64:HIS:CD2	1:A:261:VAL:H	2.04	0.63
1:C:340:TRP:HB3	3:C:382:MTT:H362	1.81	0.62
1:A:64:HIS:HE1	1:A:330:MET:O	1.82	0.62
2:D:75:ASN:N	2:D:75:ASN:HD22	1.96	0.62
1:C:72:GLN:HA	1:C:72:GLN:HE21	1.64	0.62
2:D:50:VAL:C	2:D:52:ARG:H	2.02	0.61
1:A:68:GLY:HA3	1:A:332:ASN:O	2.01	0.61
1:C:335:GLN:N	1:C:335:GLN:NE2	2.40	0.61
1:A:40:PRO:HB3	1:C:253:GLN:NE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:PRO:HB2	2:D:52:ARG:HB2	1.83	0.60
2:B:99:ASP:O	2:B:103:THR:HG22	2.02	0.60
1:A:140:LYS:HE2	4:A:506:HOH:O	2.00	0.60
1:A:295:LYS:HA	1:A:295:LYS:HE3	1.84	0.60
2:D:100:ILE:HA	2:D:104:LEU:HD22	1.83	0.60
2:B:100:ILE:HG13	2:B:104:LEU:HD22	1.84	0.60
2:D:27:TYR:O	2:D:31:VAL:HG23	2.02	0.59
2:B:52:ARG:HD2	2:B:55:GLU:OE1	2.01	0.59
2:D:5:LYS:HD2	2:D:68:TYR:CE1	2.38	0.59
2:D:101:LEU:CD2	2:D:101:LEU:H	2.14	0.58
2:B:5:LYS:HB2	2:B:5:LYS:NZ	2.17	0.58
1:C:64:HIS:CD2	1:C:261:VAL:H	2.18	0.58
2:D:19:LYS:HB2	2:D:19:LYS:NZ	2.19	0.58
1:A:296:ASP:O	1:A:297:LYS:HD3	2.04	0.58
1:C:358:ASP:O	1:C:362:LYS:HG3	2.04	0.58
1:C:115:LEU:HG	1:C:248:PRO:HD3	1.86	0.57
1:C:64:HIS:HE1	1:C:330:MET:O	1.87	0.57
1:A:43:LEU:HD13	1:A:60:ILE:HD11	1.85	0.57
2:D:102:THR:HB	2:D:104:LEU:CD1	2.35	0.57
1:C:40:PRO:HG2	1:C:43:LEU:HB3	1.85	0.57
2:D:50:VAL:HG12	2:D:51:LEU:HD13	1.85	0.57
1:A:333:ILE:HG12	1:A:335:GLN:HE21	1.69	0.57
1:A:48:PRO:HG3	1:A:70:TYR:HE1	1.68	0.57
2:B:32:LYS:CE	2:B:36:GLN:HE22	2.18	0.57
2:D:75:ASN:N	2:D:75:ASN:ND2	2.53	0.57
1:A:295:LYS:CA	1:A:295:LYS:HE3	2.35	0.56
1:C:171:TYR:OH	1:C:174:GLY:HA2	2.05	0.56
1:C:346:ALA:HB2	1:C:364:ALA:HB2	1.87	0.56
1:A:126:PRO:HB3	1:A:131:GLU:HG3	1.86	0.56
1:A:130:GLU:O	1:A:133:PRO:HD2	2.04	0.56
2:D:43:ILE:HB	2:D:90:VAL:HG13	1.87	0.56
1:C:218:ASN:HD22	1:C:218:ASN:N	2.02	0.56
1:C:54:GLY:HA3	2:D:53:LYS:NZ	2.21	0.55
2:D:14:LEU:HD12	2:D:14:LEU:C	2.26	0.55
2:D:25:LEU:HD11	2:D:81:VAL:HG11	1.88	0.55
2:D:100:ILE:HD13	2:D:101:LEU:HD22	1.88	0.55
2:D:25:LEU:N	2:D:25:LEU:HD22	2.21	0.55
2:D:13:LYS:CG	2:D:100:ILE:HG22	2.36	0.55
1:C:335:GLN:N	1:C:335:GLN:HE21	1.96	0.55
1:C:155:TYR:CB	3:C:382:MTT:H262	2.29	0.55
2:D:84:LEU:HD12	2:D:84:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HD13	1:C:275:LEU:CD1	2.37	0.54
1:A:78:GLU:OE1	1:A:102:LYS:HD2	2.07	0.54
1:C:155:TYR:HB2	3:C:382:MTT:C26	2.30	0.54
2:D:104:LEU:H	2:D:104:LEU:CD1	2.19	0.54
2:D:24:THR:CG2	2:D:91:SER:HB3	2.37	0.54
2:D:5:LYS:HB2	2:D:71:GLN:NE2	2.15	0.54
2:D:75:ASN:HD22	2:D:76:GLU:N	2.00	0.54
2:B:14:LEU:HB3	2:B:80:ALA:HB1	1.88	0.54
1:C:311:LEU:N	1:C:311:LEU:HD12	2.22	0.54
2:D:43:ILE:O	2:D:89:VAL:HA	2.08	0.54
1:A:170:LYS:HD3	1:A:180:ASP:OD1	2.08	0.54
1:A:171:TYR:OH	1:A:174:GLY:HA2	2.08	0.54
1:C:47:PHE:HB3	1:C:48:PRO:HD3	1.91	0.53
1:C:75:LEU:HD11	2:D:4:VAL:HG13	1.90	0.53
1:A:184:ASP:O	1:A:189:LYS:HE3	2.08	0.53
1:C:178:ILE:H	1:C:178:ILE:CD1	2.20	0.53
2:D:102:THR:HB	2:D:104:LEU:HD13	1.89	0.53
1:C:171:TYR:HB2	1:C:176:TYR:CE1	2.44	0.53
1:A:175:LYS:HE2	1:A:176:TYR:H	1.74	0.53
1:A:192:LEU:O	1:A:196:VAL:HG23	2.08	0.53
2:B:74:ASN:HB2	2:B:85:PHE:CE2	2.44	0.53
1:C:136:ASP:OD1	1:C:140:LYS:HE2	2.09	0.53
2:D:100:ILE:HD13	2:D:100:ILE:N	2.24	0.53
1:A:239:LYS:HZ3	1:A:239:LYS:HA	1.73	0.52
2:B:74:ASN:HD22	2:B:77:LEU:HD12	1.75	0.52
2:D:74:ASN:HD21	2:D:86:ARG:HD3	1.75	0.52
1:A:64:HIS:HD2	1:A:261:VAL:N	1.93	0.52
2:B:77:LEU:HB3	2:B:81:VAL:HG13	1.89	0.52
1:C:90:TYR:HE1	1:C:308:GLU:HG2	1.73	0.52
1:C:45:GLU:O	1:C:48:PRO:HD2	2.10	0.52
2:D:13:LYS:HG3	2:D:100:ILE:CG2	2.36	0.52
1:C:307:TYR:CE1	1:C:311:LEU:HD11	2.45	0.51
2:B:48:THR:HG22	2:B:51:LEU:HD22	1.93	0.51
2:D:86:ARG:HG3	2:D:86:ARG:HH11	1.76	0.51
2:D:43:ILE:HD12	2:D:43:ILE:N	2.26	0.51
1:A:354:ARG:O	1:A:354:ARG:HD3	2.11	0.50
1:C:232:TRP:HB2	1:C:298:PRO:HG2	1.93	0.50
1:C:307:TYR:O	1:C:311:LEU:HD13	2.11	0.50
1:A:239:LYS:HA	1:A:239:LYS:NZ	2.26	0.50
1:C:55:ASP:CG	1:C:56:GLY:H	2.14	0.50
2:B:43:ILE:HD12	2:B:92:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:HD2	1:A:326:LYS:O	2.12	0.50
1:A:43:LEU:HD13	1:A:60:ILE:CD1	2.42	0.49
1:A:220:GLY:HA2	4:A:383:HOH:O	2.11	0.49
2:D:78:GLY:N	2:D:87:VAL:HG22	2.27	0.49
1:C:177:ASP:OD1	1:C:179:LYS:HB2	2.12	0.49
1:C:274:GLU:HA	1:C:274:GLU:OE1	2.11	0.49
2:D:66:LYS:HD3	2:D:105:ALA:O	2.12	0.49
2:B:41:LEU:HD13	2:B:42:ILE:N	2.27	0.49
2:D:27:TYR:HB2	2:D:52:ARG:HH22	1.77	0.49
2:D:17:VAL:HG22	2:D:98:SER:CB	2.41	0.49
1:C:75:LEU:HD11	2:D:4:VAL:CG1	2.43	0.49
1:C:78:GLU:OE1	1:C:102:LYS:HD2	2.12	0.49
1:A:259:VAL:HB	1:A:329:ILE:HA	1.94	0.49
2:B:92:ILE:N	2:B:92:ILE:HD12	2.27	0.49
1:C:126:PRO:HB3	1:C:131:GLU:CG	2.42	0.49
2:D:18:ILE:HD11	2:D:81:VAL:HA	1.95	0.49
2:D:75:ASN:ND2	2:D:76:GLU:N	2.60	0.49
2:D:30:THR:HG23	2:D:42:ILE:HD12	1.95	0.49
2:D:77:LEU:HD22	2:D:87:VAL:CG2	2.43	0.49
1:C:220:GLY:HA2	4:C:425:HOH:O	2.13	0.48
2:D:41:LEU:HD22	2:D:43:ILE:CD1	2.43	0.48
2:D:14:LEU:HD11	2:D:80:ALA:O	2.13	0.48
1:A:18:ASN:O	1:A:22:GLU:HG2	2.13	0.48
1:A:341:TYR:HE2	3:A:382:MTT:H461	1.78	0.48
2:D:101:LEU:HD22	2:D:101:LEU:N	2.16	0.48
2:D:21:GLY:HA3	2:D:94:GLU:O	2.13	0.48
2:B:41:LEU:CD1	2:B:43:ILE:HG13	2.44	0.48
1:C:307:TYR:CZ	1:C:311:LEU:HD11	2.48	0.48
2:D:82:GLY:C	2:D:83:LYS:HD2	2.33	0.48
1:A:33:ILE:HD13	1:A:275:LEU:CD1	2.41	0.48
2:D:102:THR:HG22	2:D:103:THR:N	2.23	0.48
1:A:274:GLU:HB2	4:A:416:HOH:O	2.15	0.47
1:A:44:GLU:OE2	3:A:382:MTT:H321	2.13	0.47
2:D:49:PRO:HB2	2:D:52:ARG:CB	2.44	0.47
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.49	0.47
1:A:92:PHE:CZ	1:A:329:ILE:HD12	2.50	0.47
1:A:333:ILE:HD13	1:A:336:MET:HG2	1.97	0.47
1:C:93:THR:HB	1:C:107:PRO:HB3	1.97	0.47
1:C:126:PRO:HG3	1:C:135:LEU:HD22	1.97	0.47
1:C:6:LYS:HA	1:C:33:ILE:HG23	1.96	0.47
2:D:77:LEU:HD22	2:D:87:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:CD1	1:A:275:LEU:HD22	2.45	0.47
1:A:127:LYS:NZ	1:A:127:LYS:HB3	2.30	0.46
1:A:170:LYS:HD2	1:A:172:GLU:OE1	2.15	0.46
1:C:159:PRO:HG3	1:C:257:PRO:HA	1.97	0.46
2:D:33:SER:HA	2:D:38:LYS:CE	2.42	0.46
2:B:41:LEU:HD11	2:B:43:ILE:HG13	1.97	0.46
2:D:50:VAL:C	2:D:52:ARG:N	2.68	0.46
1:A:127:LYS:HG3	4:A:471:HOH:O	2.16	0.46
1:A:126:PRO:HG3	1:A:135:LEU:HD22	1.98	0.46
1:A:11:ILE:O	1:A:39:HIS:HA	2.16	0.46
1:C:40:PRO:HG2	1:C:43:LEU:CB	2.47	0.45
2:B:74:ASN:HA	2:B:77:LEU:HD11	1.97	0.45
2:B:78:GLY:H	2:B:81:VAL:CG1	2.29	0.45
2:D:41:LEU:HD11	2:D:105:ALA:HB3	1.97	0.45
2:D:41:LEU:HD22	2:D:43:ILE:HD12	1.98	0.45
2:D:50:VAL:O	2:D:52:ARG:N	2.49	0.45
2:D:47:ASN:O	2:D:48:THR:O	2.35	0.45
2:D:27:TYR:CE1	2:D:31:VAL:HG21	2.51	0.45
1:C:154:PRO:HD3	1:C:344:ARG:HG3	1.99	0.45
2:B:48:THR:CG2	2:B:51:LEU:HB2	2.44	0.45
2:D:75:ASN:H	2:D:75:ASN:ND2	2.15	0.45
1:A:279:PHE:O	1:A:283:TYR:HB2	2.18	0.44
1:C:340:TRP:HB3	3:C:382:MTT:C36	2.47	0.44
1:C:69:GLY:O	1:C:72:GLN:HB3	2.16	0.44
2:D:27:TYR:HB2	2:D:52:ARG:NH2	2.32	0.44
2:D:56:LEU:O	2:D:60:ALA:HB2	2.16	0.44
1:A:175:LYS:HE2	1:A:175:LYS:CA	2.45	0.44
2:D:19:LYS:HB2	2:D:19:LYS:HZ3	1.79	0.44
2:D:95:ALA:HB1	2:D:98:SER:OG	2.18	0.44
1:C:132:ILE:N	1:C:133:PRO:CD	2.81	0.44
1:C:129:TRP:CE2	1:C:160:LEU:HG	2.53	0.44
1:C:67:PHE:N	1:C:67:PHE:CD1	2.85	0.44
1:C:73:SER:HB3	2:D:4:VAL:HG12	1.99	0.44
2:D:81:VAL:HG12	2:D:81:VAL:O	2.17	0.44
1:C:260:GLY:HA2	1:C:330:MET:HE2	2.00	0.44
1:A:175:LYS:CE	1:A:176:TYR:H	2.31	0.44
1:C:12:ASN:HD22	1:C:14:ASP:CG	2.21	0.44
2:D:17:VAL:HA	2:D:20:SER:OG	2.18	0.44
2:B:103:THR:HG23	2:B:104:LEU:CD1	2.43	0.43
2:B:30:THR:HG23	2:B:91:SER:HB2	1.99	0.43
2:B:16:LEU:HD13	2:B:98:SER:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:THR:OG1	2:B:91:SER:HB3	2.18	0.43
1:C:169:PHE:CD1	1:C:178:ILE:HA	2.53	0.43
1:A:270:SER:O	1:A:273:LYS:NZ	2.51	0.43
1:A:331:PRO:HD2	1:A:336:MET:SD	2.58	0.43
2:D:87:VAL:O	2:D:87:VAL:HG23	2.18	0.43
1:A:43:LEU:C	1:A:43:LEU:HD12	2.38	0.43
2:B:62:LEU:HA	1:C:92:PHE:HB3	2.00	0.43
1:C:218:ASN:ND2	1:C:218:ASN:N	2.67	0.43
1:C:274:GLU:HB2	4:C:457:HOH:O	2.18	0.43
2:D:41:LEU:HD11	2:D:105:ALA:CB	2.48	0.43
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.53	0.43
1:A:158:TRP:N	1:A:159:PRO:CD	2.82	0.43
2:D:17:VAL:CG2	2:D:100:ILE:HD12	2.49	0.43
2:D:40:LYS:HB2	2:D:92:ILE:O	2.19	0.43
2:D:74:ASN:HD22	2:D:86:ARG:CB	2.30	0.43
1:A:254:PRO:HB3	1:A:326:LYS:HD3	2.00	0.43
1:A:33:ILE:HD13	1:A:275:LEU:HD22	2.00	0.43
2:D:58:TYR:O	2:D:61:MET:HB3	2.18	0.43
1:A:125:PRO:HA	1:A:126:PRO:HD3	1.81	0.42
1:C:181:VAL:HG12	1:C:183:VAL:HG13	2.01	0.42
1:C:254:PRO:HB3	1:C:326:LYS:HD3	2.01	0.42
1:C:311:LEU:N	1:C:311:LEU:CD1	2.82	0.42
2:B:44:ILE:HG12	2:B:89:VAL:HG13	2.01	0.42
1:C:140:LYS:HD3	1:C:144:LYS:O	2.18	0.42
1:A:317:ILE:O	1:A:321:MET:HG2	2.19	0.42
2:B:3:PRO:HB3	2:B:71:GLN:HE22	1.84	0.42
1:C:121:LEU:HA	1:C:121:LEU:HD12	1.91	0.42
1:C:11:ILE:O	1:C:39:HIS:HA	2.18	0.42
1:C:301:ALA:HA	4:C:402:HOH:O	2.18	0.42
2:D:18:ILE:HG23	2:D:23:TYR:CZ	2.54	0.42
1:C:54:GLY:HA3	2:D:53:LYS:HZ2	1.83	0.42
1:A:340:TRP:HB3	3:A:382:MTT:C36	2.48	0.42
2:B:3:PRO:CB	2:B:71:GLN:HE22	2.32	0.42
1:C:117:TYR:CE2	1:C:125:PRO:HD3	2.54	0.42
1:C:178:ILE:N	1:C:178:ILE:CD1	2.79	0.42
1:C:33:ILE:CD1	1:C:275:LEU:HD22	2.50	0.42
2:D:99:ASP:CG	2:D:104:LEU:HD21	2.40	0.42
2:D:47:ASN:OD1	2:D:48:THR:N	2.52	0.42
2:D:82:GLY:O	2:D:83:LYS:HD2	2.19	0.42
2:D:104:LEU:HD12	2:D:104:LEU:N	2.27	0.42
1:A:115:LEU:HG	1:A:248:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ASN:O	2:D:48:THR:C	2.57	0.42
1:A:159:PRO:HG3	1:A:257:PRO:HA	2.00	0.41
1:C:125:PRO:HA	1:C:126:PRO:HD3	1.83	0.41
1:A:215:ALA:O	1:A:219:LYS:HG3	2.19	0.41
1:A:291:GLU:HG3	1:A:295:LYS:HD2	2.01	0.41
1:A:340:TRP:HB3	3:A:382:MTT:H362	2.02	0.41
1:C:126:PRO:HB3	1:C:131:GLU:HG3	2.02	0.41
1:C:168:ALA:O	1:C:181:VAL:HA	2.20	0.41
1:C:177:ASP:C	1:C:179:LYS:H	2.24	0.41
2:B:16:LEU:HD23	2:B:16:LEU:HA	1.90	0.41
2:B:62:LEU:HA	1:C:92:PHE:CB	2.51	0.41
2:D:74:ASN:ND2	2:D:86:ARG:HB3	2.30	0.41
1:C:158:TRP:N	1:C:159:PRO:CD	2.84	0.41
1:C:6:LYS:HA	1:C:33:ILE:CG2	2.50	0.41
2:D:99:ASP:O	2:D:104:LEU:HD13	2.20	0.41
1:A:39:HIS:ND1	1:A:39:HIS:O	2.54	0.41
1:C:341:TYR:HE2	3:C:382:MTT:H462	1.85	0.41
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.86	0.41
1:C:171:TYR:CE1	1:C:175:LYS:N	2.89	0.40
1:A:295:LYS:N	1:A:295:LYS:HE3	2.36	0.40
2:B:103:THR:O	2:B:104:LEU:HD12	2.20	0.40
2:B:32:LYS:CE	2:B:36:GLN:NE2	2.84	0.40
2:D:22:LYS:N	2:D:94:GLU:O	2.54	0.40
2:D:17:VAL:HG22	2:D:98:SER:OG	2.21	0.40

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	366/382 (96%)	355 (97%)	10 (3%)	1 (0%)	44 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	366/382 (96%)	346 (94%)	19 (5%)	1 (0%)	44	54
2	B	102/104 (98%)	96 (94%)	5 (5%)	1 (1%)	18	19
2	D	101/104 (97%)	80 (79%)	13 (13%)	8 (8%)	1	0
All	All	935/972 (96%)	877 (94%)	47 (5%)	11 (1%)	15	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	49	PRO
2	D	4	VAL
2	D	48	THR
2	D	102	THR
1	A	173	ASN
1	C	5	GLY
2	D	49	PRO
2	D	51	LEU
2	D	103	THR
2	D	10	ILE
2	D	6	SER

### 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	293/305 (96%)	283 (97%)	10 (3%)	42	57
1	C	293/305 (96%)	283 (97%)	10 (3%)	42	57
2	B	87/87 (100%)	79 (91%)	8 (9%)	11	12
2	D	87/87 (100%)	81 (93%)	6 (7%)	18	23
All	All	760/784 (97%)	726 (96%)	34 (4%)	32	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	121	LEU
1	A	160	LEU
1	A	175	LYS
1	A	258	PHE
1	A	295	LYS
1	A	311	LEU
1	A	325	GLN
1	A	333	ILE
1	A	335	GLN
2	B	5	LYS
2	B	16	LEU
2	B	34	LEU
2	B	67	VAL
2	B	74	ASN
2	B	84	LEU
2	B	89	VAL
2	B	101	LEU
1	C	6	LYS
1	C	30	ASP
1	C	72	GLN
1	C	115	LEU
1	C	160	LEU
1	C	178	ILE
1	C	233	SER
1	C	258	PHE
1	C	325	GLN
1	C	335	GLN
2	D	12	GLN
2	D	19	LYS
2	D	25	LEU
2	D	75	ASN
2	D	100	ILE
2	D	101	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	100	ASN
1	A	173	ASN
1	A	201	ASN
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	325	GLN
1	A	335	GLN
1	A	367	ASN
2	B	36	GLN
2	B	71	GLN
2	B	74	ASN
1	C	64	HIS
1	C	72	GLN
1	C	100	ASN
1	C	173	ASN
1	C	201	ASN
1	C	218	ASN
1	C	325	GLN
1	C	335	GLN
1	C	367	ASN
2	D	12	GLN
2	D	71	GLN
2	D	75	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](#)

2 ligands 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	$\# Z  > 2$
3	MTT	A	382	-	48,48,48	1.06	4 (8%)	71,71,71	3.20	28 (39%)
3	MTT	C	382	-	48,48,48	1.06	5 (10%)	71,71,71	3.08	24 (33%)

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
3	MTT	A	382	-	-	0/20/100/100	0/4/4/4
3	MTT	C	382	-	-	0/20/100/100	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	382	MTT	O14-C14	-3.04	1.36	1.43
3	C	382	MTT	O14-C14	-2.63	1.36	1.43
3	C	382	MTT	O24-C24	-2.12	1.38	1.43
3	A	382	MTT	O24-C11	2.04	1.47	1.41
3	C	382	MTT	O24-C11	2.12	1.47	1.41
3	C	382	MTT	C33-C34	2.24	1.58	1.52
3	A	382	MTT	C33-C34	2.30	1.58	1.52
3	C	382	MTT	O43-C43	2.31	1.48	1.43
3	A	382	MTT	O43-C43	2.38	1.48	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	382	MTT	C11-O24-C24	-10.43	92.58	118.00
3	C	382	MTT	C11-O24-C24	-9.63	94.53	118.00
3	C	382	MTT	C21-O34-C34	-8.20	98.02	118.00
3	A	382	MTT	C21-O34-C34	-8.11	98.23	118.00
3	C	382	MTT	O35-C35-C34	-4.00	101.56	109.75
3	A	382	MTT	O35-C35-C34	-3.60	102.38	109.75
3	C	382	MTT	C33-C34-C35	-2.62	105.31	110.88
3	A	382	MTT	C33-C34-C35	-2.58	105.41	110.88
3	A	382	MTT	O13-C13-C14	2.11	114.96	110.36
3	A	382	MTT	O24-C24-C25	2.15	114.63	109.34
3	C	382	MTT	C26-C25-C24	2.16	119.12	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	382	MTT	O41-C41-C42	2.19	115.61	109.42
3	A	382	MTT	C26-C25-C24	2.28	119.46	113.24
3	A	382	MTT	O15-C11-C12	2.31	114.76	110.30
3	A	382	MTT	O45-C41-C42	2.55	114.27	110.04
3	C	382	MTT	O45-C41-C42	2.59	114.34	110.04
3	C	382	MTT	C32-C33-C34	2.63	115.06	109.61
3	A	382	MTT	C32-C33-C34	2.68	115.16	109.61
3	C	382	MTT	C11-O15-C15	2.80	119.00	113.72
3	A	382	MTT	C42-C43-C44	2.83	115.47	109.61
3	C	382	MTT	C42-C43-C44	2.86	115.54	109.61
3	A	382	MTT	C11-O15-C15	2.88	119.13	113.72
3	C	382	MTT	C11-C12-C13	2.95	115.46	109.98
3	A	382	MTT	C21-C22-C23	3.02	115.59	109.98
3	C	382	MTT	C36-C35-C34	3.10	121.68	113.24
3	C	382	MTT	C21-C22-C23	3.12	115.77	109.98
3	A	382	MTT	O25-C21-C22	3.19	116.44	110.30
3	C	382	MTT	O25-C21-C22	3.21	116.49	110.30
3	A	382	MTT	C36-C35-C34	3.26	122.12	113.24
3	A	382	MTT	C11-C12-C13	3.26	116.04	109.98
3	C	382	MTT	O12-C12-C13	3.55	118.07	110.36
3	A	382	MTT	O12-C12-C13	3.71	118.43	110.36
3	A	382	MTT	C41-C42-C43	4.03	117.93	110.65
3	C	382	MTT	O35-C31-C32	4.06	118.12	110.30
3	C	382	MTT	C41-C42-C43	4.06	117.98	110.65
3	C	382	MTT	C21-O25-C25	4.26	121.73	113.72
3	C	382	MTT	O23-C23-C24	4.27	119.58	109.87
3	A	382	MTT	O34-C34-C35	4.29	119.90	109.34
3	C	382	MTT	O34-C34-C35	4.33	120.00	109.34
3	A	382	MTT	O35-C31-C32	4.36	118.70	110.30
3	A	382	MTT	O23-C23-C24	4.46	120.02	109.87
3	A	382	MTT	C21-O25-C25	4.53	122.26	113.72
3	C	382	MTT	O22-C22-C23	5.06	121.37	110.36
3	A	382	MTT	O22-C22-C23	5.10	121.44	110.36
3	A	382	MTT	C31-O35-C35	5.34	123.77	113.72
3	C	382	MTT	C31-O35-C35	5.40	123.90	113.72
3	C	382	MTT	C41-O45-C45	6.04	124.29	113.39
3	A	382	MTT	C41-O45-C45	6.05	124.31	113.39
3	C	382	MTT	O24-C11-C12	7.38	124.74	108.11
3	A	382	MTT	O24-C11-C12	8.24	126.68	108.11
3	C	382	MTT	O34-C21-C22	10.65	132.12	108.11
3	A	382	MTT	O34-C21-C22	10.90	132.68	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	382	MTT	7	0
3	C	382	MTT	7	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.