



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:45 PM GMT

PDB ID : 1QI4  
Title : MUTANT (E219G) MALTOTETRAOSE-FORMING EXO-AMYLASE IN  
COMPLEX WITH MALTOTETRAOSE  
Authors : Hasegawa, K.; Kubota, M.; Matsuura, Y.  
Deposited on : 1999-06-01  
Resolution : 2.00 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

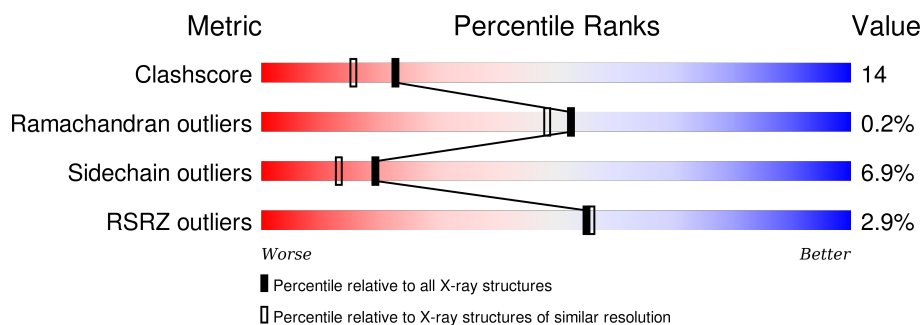
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	429	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3491 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 PROTEIN (EXO-MALTOTETRAOHYDROLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3292	2067	596	619	10			

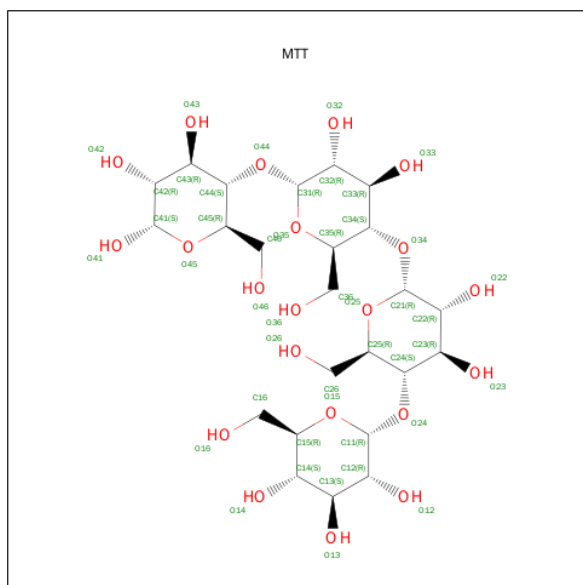
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	GLU	ENGINEERED	UNP P13507

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is MALTOTETRAOSE (three-letter code: MTT) (formula: C<sub>24</sub>H<sub>42</sub>O<sub>21</sub>).



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

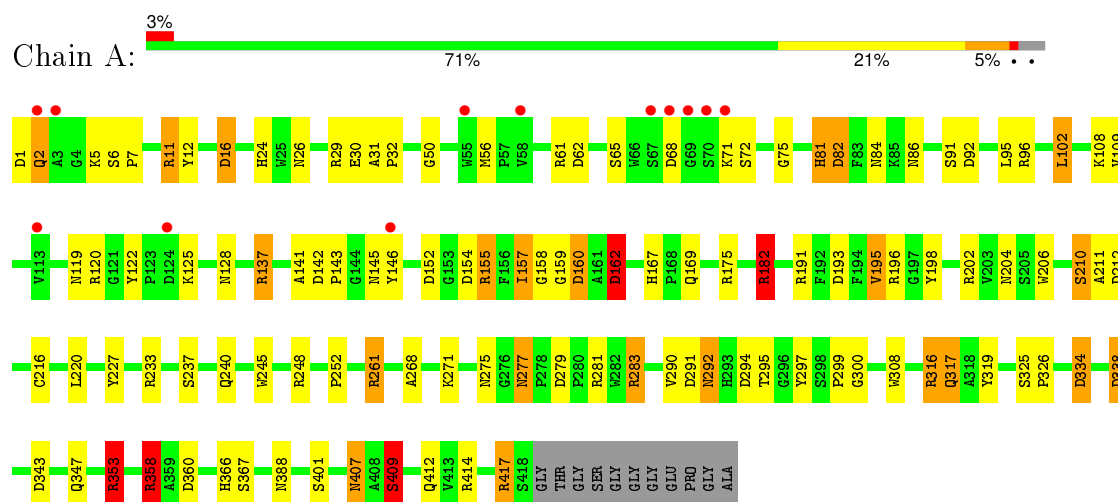
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PROTEIN (EXO-MALTOTETRAOHYDROLASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.52Å 171.10Å 46.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 34.86 – 1.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 87.4 (34.86-1.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.00Å)	Xtriage
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.180 , (Not available) 0.164 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 32330 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.87	1/3397 (0.0%)	1.77	63/4624 (1.4%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ASP	CA-CB	6.22	1.67	1.53

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	CD-NE-CZ	40.19	179.86	123.60
1	A	175	ARG	NE-CZ-NH2	20.94	130.77	120.30
1	A	353	ARG	NE-CZ-NH1	15.68	128.14	120.30
1	A	82	ASP	CB-CG-OD1	-15.53	104.32	118.30
1	A	353	ARG	NE-CZ-NH2	-14.47	113.07	120.30
1	A	11	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	A	137	ARG	NE-CZ-NH1	13.07	126.83	120.30
1	A	417	ARG	NE-CZ-NH1	12.51	126.55	120.30
1	A	182	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	A	283	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	A	120	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	A	82	ASP	CB-CG-OD2	9.85	127.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	A	182	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	A	155	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	82	ASP	CB-CA-C	-8.24	93.91	110.40
1	A	233	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	281	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	338	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	175	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	A	334	ASP	CA-CB-CG	-7.32	97.29	113.40
1	A	248	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	A	120	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	191	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	137	ARG	CD-NE-CZ	6.75	133.05	123.60
1	A	152	ASP	CB-CG-OD1	6.65	124.28	118.30
1	A	409	SER	N-CA-CB	6.63	120.44	110.50
1	A	291	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	343	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	319	TYR	CB-CG-CD1	-6.44	117.13	121.00
1	A	11	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	155	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	300	GLY	C-N-CA	6.25	137.31	121.70
1	A	195	VAL	CB-CA-C	6.23	123.24	111.40
1	A	196	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	A	82	ASP	CA-CB-CG	-6.15	99.87	113.40
1	A	212	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	175	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
1	A	198	TYR	CB-CG-CD2	6.08	124.65	121.00
1	A	347	GLN	CA-CB-CG	6.05	126.71	113.40
1	A	347	GLN	N-CA-CB	6.04	121.47	110.60
1	A	360	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	414	ARG	CD-NE-CZ	6.01	132.02	123.60
1	A	316	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	16	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	96	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	160	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	162	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	102	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	261	ARG	CD-NE-CZ	5.58	131.41	123.60
1	A	297	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	290	VAL	CA-CB-CG1	5.55	119.22	110.90
1	A	261	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	A	360	ASP	CB-CG-OD2	-5.33	113.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	HIS	C-N-CA	5.31	134.97	121.70
1	A	195	VAL	CA-CB-CG1	5.25	118.77	110.90
1	A	227	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	414	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	358	ARG	CD-NE-CZ	-5.21	116.31	123.60
1	A	142	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	122	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	366	HIS	C-N-CA	5.04	134.31	121.70
1	A	212	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	ARG	Sidechain

## 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	3292	0	3010	85	0
2	A	2	0	0	0	0
3	A	45	0	41	4	0
4	A	152	0	0	3	0
All	All	3491	0	3051	86	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 14.

All (86) 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:11:ARG:HH12	1:A:204:ASN:HD22	1.10	0.99
1:A:299:PRO:HD3	1:A:334:ASP:OD2	1.71	0.91
1:A:167:HIS:HD2	1:A:169:GLN:H	1.16	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:SER:H	1:A:240:GLN:HE21	1.15	0.88
1:A:193:ASP:OD1	3:A:460:MTT:H411	1.73	0.87
1:A:277:ASN:HD22	1:A:279:ASP:H	1.26	0.80
1:A:317:GLN:H	1:A:317:GLN:HE21	1.29	0.80
1:A:167:HIS:CD2	1:A:169:GLN:H	1.99	0.80
1:A:237:SER:H	1:A:240:GLN:NE2	1.83	0.76
1:A:26:ASN:HD22	1:A:29:ARG:HE	1.33	0.75
1:A:334:ASP:OD1	1:A:338:ASP:OD2	2.06	0.72
1:A:11:ARG:HH12	1:A:204:ASN:ND2	1.88	0.69
1:A:145:ASN:ND2	1:A:155:ARG:H	1.90	0.69
1:A:86:ASN:ND2	1:A:92:ASP:H	1.91	0.69
1:A:182:ARG:HD2	1:A:211:ALA:HB2	1.73	0.69
1:A:407:ASN:C	1:A:407:ASN:HD22	1.97	0.68
1:A:82:ASP:HB3	1:A:84:ASN:H	1.57	0.68
1:A:26:ASN:ND2	1:A:29:ARG:HE	1.92	0.66
1:A:81:HIS:HD2	4:A:508:HOH:O	1.79	0.64
1:A:216:CYS:O	1:A:252:PRO:HD2	1.99	0.63
1:A:292:ASN:HD21	1:A:294:ASP:HB2	1.65	0.61
1:A:325:SER:HB2	1:A:326:PRO:HD2	1.82	0.61
1:A:11:ARG:HH22	1:A:204:ASN:ND2	1.99	0.60
1:A:1:ASP:OD2	1:A:108:LYS:NZ	2.34	0.60
1:A:24:HIS:HD2	1:A:26:ASN:H	1.50	0.60
1:A:11:ARG:NH1	1:A:204:ASN:HD22	1.91	0.59
1:A:292:ASN:ND2	1:A:295:THR:H	1.99	0.59
1:A:277:ASN:ND2	1:A:279:ASP:H	1.97	0.59
1:A:145:ASN:HD21	1:A:154:ASP:HB3	1.68	0.58
1:A:325:SER:HB2	1:A:326:PRO:CD	2.33	0.58
1:A:167:HIS:HD2	1:A:169:GLN:N	1.95	0.58
1:A:31:ALA:N	1:A:32:PRO:HD3	2.19	0.58
1:A:195:VAL:HG13	1:A:245:TRP:NE1	2.20	0.56
1:A:50:GLY:HA2	1:A:353:ARG:NH2	2.21	0.56
1:A:317:GLN:NE2	1:A:317:GLN:H	2.00	0.56
1:A:26:ASN:HD22	1:A:29:ARG:NE	2.04	0.55
1:A:145:ASN:HD21	1:A:155:ARG:H	1.53	0.55
1:A:292:ASN:HD22	1:A:292:ASN:C	2.11	0.54
1:A:316:ARG:HH11	1:A:316:ARG:HG3	1.73	0.53
1:A:299:PRO:CD	1:A:334:ASP:OD2	2.52	0.52
1:A:86:ASN:ND2	1:A:91:SER:HB2	2.24	0.52
1:A:141:ALA:O	1:A:143:PRO:HD3	2.10	0.52
1:A:353:ARG:HD3	4:A:746:HOH:O	2.11	0.51
1:A:155:ARG:HB2	1:A:159:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:C	1:A:32:PRO:HD3	2.31	0.51
1:A:195:VAL:HG12	1:A:220:LEU:HB2	1.94	0.50
1:A:292:ASN:ND2	1:A:294:ASP:H	2.10	0.49
1:A:277:ASN:O	1:A:283:ARG:HD3	2.11	0.49
1:A:68:ASP:O	1:A:68:ASP:OD1	2.31	0.48
1:A:155:ARG:HA	1:A:162:ASP:OD2	2.13	0.48
1:A:388:ASN:ND2	1:A:412:GLN:HB3	2.29	0.47
1:A:50:GLY:CA	1:A:353:ARG:NH2	2.77	0.47
1:A:409:SER:O	1:A:412:GLN:HG3	2.16	0.46
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.41	0.46
1:A:268:ALA:O	1:A:271:LYS:HG2	2.16	0.46
1:A:202:ARG:HG2	1:A:206:TRP:CZ3	2.50	0.46
1:A:155:ARG:HD2	1:A:159:GLY:HA3	1.98	0.45
1:A:125:LYS:NZ	1:A:128:ASN:ND2	2.64	0.45
1:A:237:SER:N	1:A:240:GLN:HE21	1.98	0.45
1:A:157:ILE:HG21	3:A:460:MTT:H131	1.99	0.45
1:A:31:ALA:N	1:A:32:PRO:CD	2.79	0.44
1:A:388:ASN:HD22	1:A:412:GLN:HB3	1.83	0.44
1:A:86:ASN:HD22	1:A:91:SER:CB	2.30	0.44
1:A:182:ARG:HD2	1:A:211:ALA:CB	2.42	0.44
1:A:125:LYS:HZ3	1:A:128:ASN:HD21	1.66	0.44
3:A:460:MTT:C11	3:A:460:MTT:H261	2.48	0.43
1:A:6:SER:HB2	1:A:7:PRO:CD	2.47	0.43
1:A:62:ASP:O	1:A:75:GLY:HA2	2.19	0.43
1:A:125:LYS:HZ3	1:A:128:ASN:ND2	2.17	0.43
1:A:316:ARG:NH1	1:A:316:ARG:HG3	2.33	0.43
1:A:137:ARG:NH2	1:A:146:TYR:O	2.42	0.43
1:A:167:HIS:CD2	1:A:169:GLN:HB3	2.54	0.42
1:A:24:HIS:HE1	4:A:732:HOH:O	2.01	0.42
1:A:409:SER:HB2	1:A:412:GLN:HE21	1.83	0.42
1:A:193:ASP:OD1	3:A:460:MTT:C41	2.57	0.42
1:A:2:GLN:HB2	1:A:16:ASP:OD2	2.19	0.42
1:A:157:ILE:HG22	1:A:158:GLY:N	2.34	0.42
1:A:407:ASN:C	1:A:407:ASN:ND2	2.67	0.42
1:A:358:ARG:HD2	1:A:358:ARG:HH11	1.67	0.42
1:A:261:ARG:NE	1:A:261:ARG:HA	2.34	0.41
1:A:292:ASN:ND2	1:A:294:ASP:HB2	2.34	0.41
1:A:160:ASP:N	1:A:160:ASP:OD1	2.49	0.41
1:A:50:GLY:HA2	1:A:353:ARG:HH22	1.84	0.41
1:A:86:ASN:HD22	1:A:91:SER:HB2	1.85	0.41
1:A:182:ARG:HD3	1:A:210:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:HG3	1:A:109:VAL:HG13	2.03	0.41

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	416/429 (97%)	400 (96%)	15 (4%)	1 (0%)	52 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ILE

### 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	332/336 (99%)	309 (93%)	23 (7%)	19 13

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	5	LYS

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Mol	Chain	Res	Type
1	A	12	TYR
1	A	65	SER
1	A	71	LYS
1	A	72	SER
1	A	95	LEU
1	A	102	LEU
1	A	119	ASN
1	A	162	ASP
1	A	210	SER
1	A	275	ASN
1	A	277	ASN
1	A	292	ASN
1	A	308	TRP
1	A	317	GLN
1	A	353	ARG
1	A	358	ARG
1	A	367	SER
1	A	401	SER
1	A	407	ASN
1	A	409	SER
1	A	417	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	24	HIS
1	A	26	ASN
1	A	81	HIS
1	A	86	ASN
1	A	119	ASN
1	A	128	ASN
1	A	145	ASN
1	A	167	HIS
1	A	204	ASN
1	A	240	GLN
1	A	277	ASN
1	A	292	ASN
1	A	317	GLN
1	A	335	HIS
1	A	347	GLN
1	A	366	HIS

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Mol	Chain	Res	Type
1	A	388	ASN
1	A	407	ASN
1	A	412	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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$
3	MTT	A	460	-	48,48,48	0.90	3 (6%)	71,71,71	1.78	12 (16%)

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	460	-	-	0/20/100/100	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	460	MTT	C41-C42	-2.88	1.47	1.52
3	A	460	MTT	O34-C34	-2.36	1.37	1.43
3	A	460	MTT	O45-C41	-2.35	1.38	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	MTT	O43-C43-C42	-3.85	101.67	110.34
3	A	460	MTT	O24-C11-C12	2.19	113.44	108.10
3	A	460	MTT	C31-O44-C44	2.30	124.02	118.01
3	A	460	MTT	C21-O34-C34	2.32	124.06	118.01
3	A	460	MTT	C41-C42-C43	2.41	114.02	110.43
3	A	460	MTT	O34-C34-C35	2.41	115.67	109.32
3	A	460	MTT	C11-C12-C13	2.47	114.85	109.97
3	A	460	MTT	O41-C41-O45	2.55	117.23	110.25
3	A	460	MTT	O42-C42-C41	2.95	116.33	109.82
3	A	460	MTT	O34-C21-C22	4.46	118.95	108.10
3	A	460	MTT	O45-C41-C42	5.92	119.25	109.80
3	A	460	MTT	C41-O45-C45	7.16	126.72	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	460	MTT	4	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	418/429 (97%)	-0.30	12 (2%) 55 56	10, 18, 33, 48	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	TYR	5.7
1	A	124	ASP	3.9
1	A	2	GLN	3.4
1	A	71	LYS	3.0
1	A	70	SER	3.0
1	A	3	ALA	2.9
1	A	58	VAL	2.5
1	A	68	ASP	2.4
1	A	67	SER	2.2
1	A	69	GLY	2.1
1	A	55	TRP	2.1
1	A	113	VAL	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 carbohydrates 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. 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(Å <sup>2</sup> )	Q<0.9
3	MTT	A	460	45/45	0.93	0.10	-0.39	15,18,24,26	0
2	CA	A	452	1/1	1.00	0.03	-1.19	17,17,17,17	0
2	CA	A	451	1/1	0.99	0.05	-1.58	19,19,19,19	0

## 6.5 Other polymers

There are no such residues in this entry.