



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:23 pm BST

PDB ID : 2XUW  
Title : Crystal Structure of Apolaccase from *Thermus thermophilus* HB27  
Authors : Serrano-Posada, H.; Valderrama, B.; Rudino-Pinera, E.  
Deposited on : 2010-10-21  
Resolution : 1.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

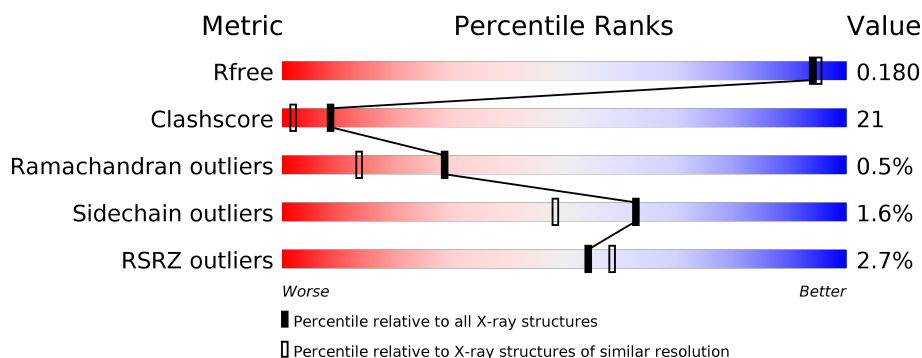
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	439	<div> <div>3%</div> <div>80%</div> <div>18%</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
2	MPD	A	1470	-	X	-	-
2	MPD	A	1474	X	X	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	1475	-	-	X	-
2	MPD	A	1478	-	-	X	X
3	MRD	A	1476	X	-	X	-
3	MRD	A	1477	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4698 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.

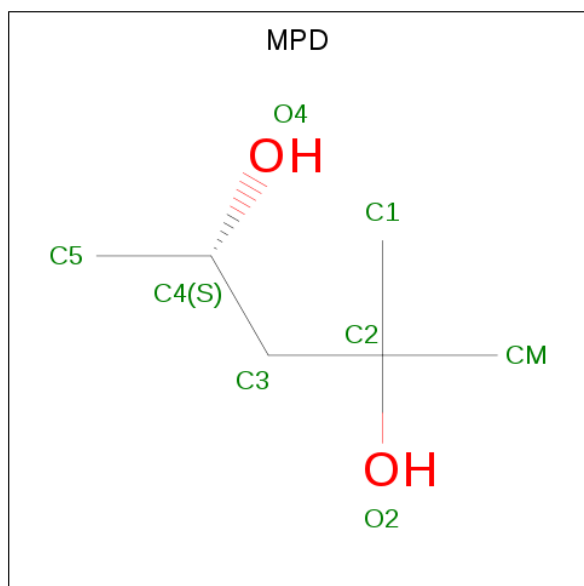
- Molecule 1 is a protein called LACCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	4045	2599	729	700	17	0	65	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	LEU	SEE REMARK 999	UNP Q72HW2

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



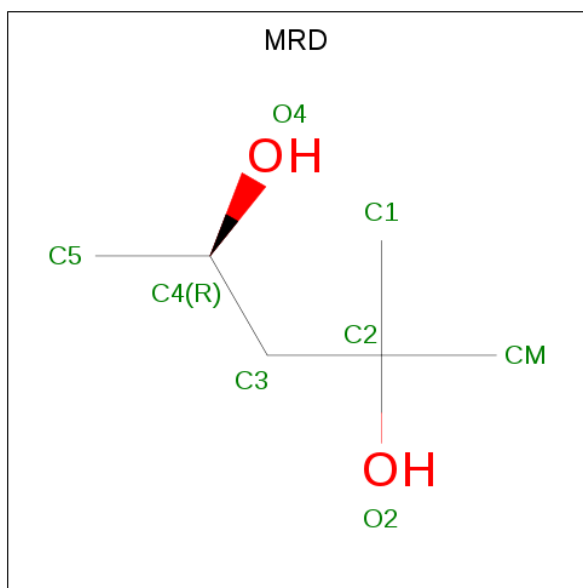
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	8	6	2	0	0
2	A	1	8	6	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		

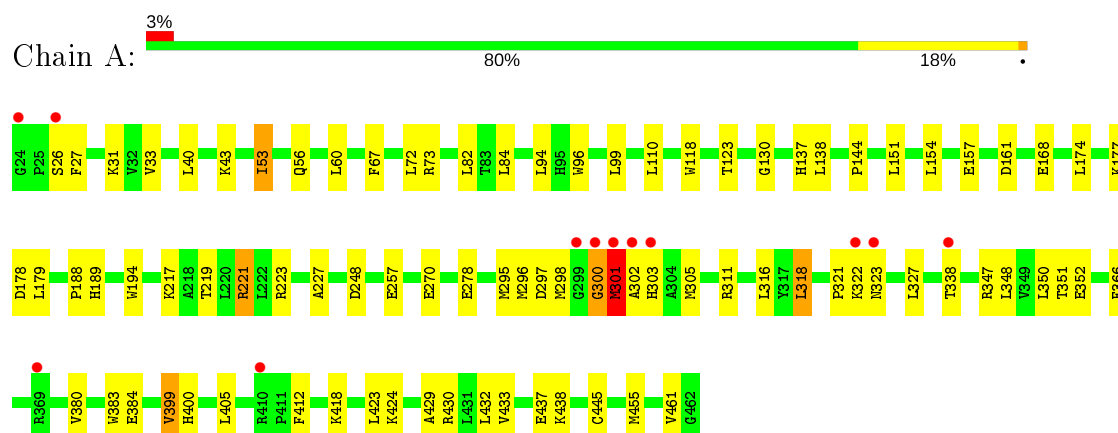
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	525	Total	O	0	0
			525	525		

### 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.

#### • Molecule 1: LACCASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.02Å 110.12Å 96.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.47 – 1.70 27.53 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (26.47-1.70) 99.0 (27.53-1.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.71Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.151 , 0.185 0.145 , 0.180	Depositor DCC
$R_{free}$ test set	2747 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, MPD

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	0.48	0/4147	0.61	1/5650 (0.0%)

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	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	301	MET	N-CA-CB	-7.98	96.23	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	300	GLY	Mainchain,Peptide
1	A	347[B]	ARG	Mainchain

### 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	4045	0	4137	134	0
2	A	72	0	122	50	0
3	A	56	0	97	28	0
4	A	525	0	0	33	1
All	All	4698	0	4356	176	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 21.

All (176) 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)
2:A:1475:MPD:CM	2:A:1478:MPD:H13	1.50	1.40
1:A:194:TRP:HZ2	2:A:1474:MPD:C5	1.42	1.29
1:A:194:TRP:CZ2	2:A:1474:MPD:C5	2.33	1.10
2:A:1475:MPD:CM	2:A:1478:MPD:C1	2.31	1.08
1:A:194:TRP:HZ2	2:A:1474:MPD:H51	1.19	1.07
2:A:1475:MPD:HM3	2:A:1478:MPD:H13	1.23	1.06
1:A:189:HIS:H	2:A:1474:MPD:CM	1.66	1.06
3:A:1476:MRD:H1C1	3:A:1476:MRD:H5C2	1.37	1.03
1:A:189:HIS:HB2	2:A:1474:MPD:HM1	1.39	1.02
1:A:327[B]:LEU:HD11	4:A:2237:HOH:O	1.59	1.01
3:A:1476:MRD:C5	3:A:1476:MRD:C1	2.39	1.01
1:A:300:GLY:O	1:A:301:MET:O	1.79	1.00
2:A:1475:MPD:HM1	2:A:1478:MPD:H13	1.41	0.99
1:A:144:PRO:HG3	2:A:1474:MPD:H52	1.39	0.99
1:A:194:TRP:HZ2	2:A:1474:MPD:H53	1.24	0.98
1:A:194:TRP:CZ2	2:A:1474:MPD:H53	1.98	0.98
2:A:1475:MPD:H11	2:A:1475:MPD:O4	1.65	0.96
3:A:1476:MRD:H1C3	3:A:1476:MRD:H5C3	1.45	0.95
1:A:123[B]:THR:OG1	2:A:1475:MPD:H32	1.68	0.93
3:A:1476:MRD:H1C1	3:A:1476:MRD:C5	1.99	0.91
1:A:194:TRP:CZ2	2:A:1474:MPD:H51	2.04	0.91
1:A:189:HIS:CB	2:A:1474:MPD:HM1	2.00	0.90
1:A:123[A]:THR:HB	2:A:1475:MPD:H32	1.53	0.90
1:A:338:THR:O	4:A:2398:HOH:O	1.89	0.89
3:A:1468:MRD:H5C2	3:A:1468:MRD:HMC1	1.55	0.88
1:A:438:LYS:HA	1:A:461[B]:VAL:HG13	1.55	0.88
2:A:1475:MPD:HM2	4:A:2500:HOH:O	1.75	0.86
3:A:1473:MRD:H1C1	3:A:1473:MRD:O4	1.75	0.86
3:A:1476:MRD:C1	3:A:1476:MRD:H5C3	2.02	0.86
1:A:67[C]:PHE:HZ	1:A:177[C]:LYS:HD2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56[A]:GLN:NE2	4:A:2083:HOH:O	2.07	0.85
3:A:1468:MRD:CM	3:A:1468:MRD:H5C2	2.07	0.85
1:A:423[A]:LEU:HD21	1:A:429:ALA:HB2	1.60	0.83
1:A:189:HIS:H	2:A:1474:MPD:HM3	1.41	0.83
1:A:278[B]:GLU:HG2	4:A:2379:HOH:O	1.79	0.82
1:A:189:HIS:H	2:A:1474:MPD:HM1	1.45	0.81
2:A:1475:MPD:HM3	2:A:1478:MPD:C1	2.04	0.81
3:A:1466:MRD:H5C2	3:A:1473:MRD:H1C3	1.63	0.81
1:A:327[B]:LEU:H	1:A:327[B]:LEU:CD1	1.96	0.79
1:A:189:HIS:N	2:A:1474:MPD:CM	2.45	0.78
2:A:1475:MPD:O4	2:A:1475:MPD:C1	2.30	0.78
1:A:161:ASP:OD1	4:A:2231:HOH:O	2.01	0.78
1:A:296:MET:HE3	1:A:305:MET:HG3	1.65	0.78
1:A:437:GLU:O	1:A:461[B]:VAL:HG11	1.84	0.78
1:A:327[B]:LEU:H	1:A:327[B]:LEU:HD13	1.47	0.77
1:A:26[B]:SER:HB2	4:A:2007:HOH:O	1.87	0.75
3:A:1477:MRD:CM	4:A:2324:HOH:O	2.34	0.74
3:A:1469:MRD:H5C3	2:A:1474:MPD:O4	1.87	0.74
1:A:366:PHE:CE2	3:A:1476:MRD:H3C1	2.23	0.74
1:A:144:PRO:CG	2:A:1474:MPD:H52	2.17	0.73
2:A:1471:MPD:C5	4:A:2394:HOH:O	2.37	0.73
1:A:189:HIS:N	2:A:1474:MPD:HM3	2.04	0.71
3:A:1477:MRD:H1C1	4:A:2308:HOH:O	1.91	0.70
2:A:1471:MPD:H53	4:A:2394:HOH:O	1.91	0.70
1:A:67[C]:PHE:CZ	1:A:177[C]:LYS:HD2	2.26	0.69
1:A:461[B]:VAL:HG12	4:A:2498:HOH:O	1.92	0.69
1:A:123[B]:THR:HG1	2:A:1475:MPD:H32	1.58	0.69
1:A:161:ASP:CG	4:A:2231:HOH:O	2.32	0.67
1:A:298[B]:MET:HB2	1:A:301:MET:HE3	1.78	0.66
1:A:298[A]:MET:H	1:A:301:MET:HG3	1.61	0.65
1:A:432[B]:LEU:HD23	1:A:432[B]:LEU:C	2.15	0.65
1:A:384:GLU:HG2	1:A:430[B]:ARG:HG2	1.79	0.65
1:A:298[B]:MET:H	1:A:301:MET:HG3	1.61	0.65
3:A:1477:MRD:HMC3	4:A:2324:HOH:O	1.97	0.65
1:A:73[A]:ARG:HD3	1:A:157[A]:GLU:OE2	1.99	0.63
1:A:189:HIS:N	2:A:1474:MPD:HM1	2.12	0.63
1:A:437:GLU:OE1	2:A:1478:MPD:HM3	1.98	0.62
1:A:53[B]:ILE:HD11	1:A:179:LEU:HD23	1.82	0.62
2:A:1475:MPD:H13	4:A:2146:HOH:O	1.98	0.62
1:A:123[A]:THR:O	2:A:1475:MPD:H12	1.99	0.62
1:A:26[A]:SER:HB3	4:A:2007:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:HA	1:A:301:MET:HB3	1.81	0.61
1:A:327[B]:LEU:N	1:A:327[B]:LEU:CD1	2.59	0.61
3:A:1473:MRD:O4	3:A:1473:MRD:C1	2.48	0.61
1:A:295:MET:CG	3:A:1466:MRD:HMC3	2.32	0.60
1:A:423[A]:LEU:HD21	1:A:429:ALA:CB	2.29	0.60
1:A:278[A]:GLU:OE2	1:A:322:LYS:HG3	2.01	0.60
1:A:219:THR:OG1	1:A:327[B]:LEU:HD13	2.01	0.60
1:A:437:GLU:O	1:A:461[B]:VAL:CG1	2.50	0.60
1:A:399[B]:VAL:HG23	1:A:400:HIS:CD2	2.37	0.60
1:A:99[B]:LEU:HD13	4:A:2202:HOH:O	2.02	0.60
1:A:380:VAL:HG11	1:A:432[B]:LEU:HD21	1.84	0.59
1:A:424[A]:LYS:HE3	4:A:2483:HOH:O	2.01	0.59
1:A:82[B]:LEU:HD22	1:A:96:TRP:CH2	2.37	0.59
1:A:53[A]:ILE:HD13	1:A:60[A]:LEU:HD11	1.86	0.58
1:A:366:PHE:CZ	3:A:1476:MRD:H3C1	2.38	0.58
1:A:295:MET:HG3	3:A:1466:MRD:HMC3	1.86	0.58
2:A:1475:MPD:HM3	4:A:2146:HOH:O	2.04	0.56
2:A:1475:MPD:HM1	2:A:1478:MPD:C1	2.20	0.56
2:A:1475:MPD:HM2	2:A:1478:MPD:C1	2.33	0.55
1:A:130:GLY:HA2	4:A:2338:HOH:O	2.05	0.55
2:A:1471:MPD:H51	4:A:2394:HOH:O	2.04	0.55
1:A:123[B]:THR:O	2:A:1475:MPD:H12	2.07	0.54
2:A:1474:MPD:HM3	4:A:2253:HOH:O	2.06	0.54
1:A:461[B]:VAL:CG1	4:A:2498:HOH:O	2.53	0.54
1:A:96:TRP:HB3	1:A:99[A]:LEU:HD12	1.89	0.54
1:A:110[A]:LEU:O	1:A:138[A]:LEU:HD21	2.08	0.53
1:A:72:LEU:HB2	1:A:154[B]:LEU:HD13	1.90	0.53
1:A:223[A]:ARG:NH1	1:A:270:GLU:OE2	2.42	0.52
1:A:189:HIS:CG	2:A:1474:MPD:HM1	2.45	0.51
1:A:366:PHE:HE2	3:A:1476:MRD:H3C1	1.70	0.51
1:A:405:LEU:HD11	1:A:432[A]:LEU:HG	1.91	0.51
3:A:1477:MRD:HMC1	4:A:2324:HOH:O	2.08	0.50
1:A:327[B]:LEU:HD12	1:A:327[B]:LEU:N	2.26	0.50
1:A:84:LEU:HD22	1:A:94[A]:LEU:HG	1.94	0.50
1:A:110[B]:LEU:HD11	1:A:118:TRP:CE2	2.46	0.50
3:A:1468:MRD:C5	3:A:1468:MRD:HMC1	2.31	0.49
1:A:137:HIS:HD2	4:A:2204:HOH:O	1.94	0.49
3:A:1468:MRD:CM	3:A:1468:MRD:C5	2.78	0.49
1:A:82[B]:LEU:HD22	1:A:96:TRP:HH2	1.76	0.49
1:A:350[B]:LEU:HD12	1:A:350[B]:LEU:N	2.27	0.49
1:A:123[A]:THR:HB	2:A:1475:MPD:C3	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223[C]:ARG:NH2	4:A:2293:HOH:O	2.40	0.49
1:A:123[A]:THR:H	2:A:1475:MPD:H12	1.77	0.49
3:A:1468:MRD:HMC3	3:A:1468:MRD:H5C2	1.92	0.49
1:A:168:GLU:O	1:A:217[A]:LYS:HD3	2.13	0.48
1:A:296:MET:HG2	1:A:298[A]:MET:HG2	1.94	0.48
1:A:27:PHE:HZ	1:A:174[B]:LEU:HD22	1.78	0.48
1:A:278[A]:GLU:HG2	1:A:322:LYS:HA	1.94	0.47
1:A:424[A]:LYS:CE	4:A:2483:HOH:O	2.60	0.47
1:A:110[B]:LEU:C	1:A:110[B]:LEU:HD23	2.34	0.47
1:A:123[B]:THR:H	2:A:1475:MPD:H12	1.79	0.47
1:A:296:MET:HE3	1:A:305:MET:CG	2.42	0.47
1:A:383:TRP:CD1	1:A:433[B]:VAL:HG11	2.50	0.47
1:A:33:VAL:HG12	1:A:40[B]:LEU:HD21	1.96	0.47
3:A:1469:MRD:H1C3	3:A:1469:MRD:H4	1.73	0.46
1:A:53[B]:ILE:O	1:A:56[B]:GLN:HG3	2.16	0.46
2:A:1478:MPD:C1	4:A:2500:HOH:O	2.63	0.46
1:A:189:HIS:ND1	2:A:1474:MPD:CM	2.78	0.46
1:A:53[C]:ILE:HG21	1:A:53[C]:ILE:HD13	1.42	0.46
1:A:31:LYS:HD3	2:A:1472:MPD:H4	1.97	0.45
1:A:300:GLY:O	1:A:301:MET:C	2.49	0.45
1:A:53[B]:ILE:O	1:A:56[B]:GLN:CG	2.65	0.45
1:A:257[B]:GLU:HG3	4:A:2328:HOH:O	2.17	0.45
1:A:298[A]:MET:HB2	1:A:301:MET:CE	2.47	0.45
1:A:278[A]:GLU:CD	1:A:322:LYS:HA	2.37	0.45
1:A:300:GLY:H	1:A:301:MET:HB2	1.82	0.44
1:A:338:THR:HA	4:A:2397:HOH:O	2.16	0.44
1:A:151[B]:LEU:HD22	1:A:151[B]:LEU:C	2.37	0.44
1:A:298[A]:MET:CG	1:A:301:MET:HE3	2.47	0.44
1:A:298[B]:MET:HB2	1:A:301:MET:CE	2.45	0.43
1:A:188:PRO:HA	2:A:1474:MPD:HM3	1.99	0.43
1:A:177[C]:LYS:HD3	1:A:178:ASP:O	2.19	0.43
1:A:257[B]:GLU:HG3	1:A:257[B]:GLU:O	2.18	0.43
1:A:278[A]:GLU:CG	1:A:322:LYS:HA	2.49	0.43
1:A:27:PHE:HZ	1:A:174[B]:LEU:CD2	2.32	0.42
1:A:316:LEU:C	1:A:316:LEU:HD12	2.40	0.42
1:A:445:CYS:HB2	1:A:455[A]:MET:SD	2.60	0.42
1:A:73[A]:ARG:NH1	1:A:157[A]:GLU:HG2	2.35	0.42
1:A:348[B]:LEU:HD12	1:A:348[B]:LEU:N	2.35	0.42
1:A:53[C]:ILE:HG23	1:A:53[C]:ILE:O	2.20	0.42
2:A:1470:MPD:H4	4:A:2521:HOH:O	2.20	0.41
1:A:53[B]:ILE:HD12	1:A:53[B]:ILE:HG21	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177[D]:LYS:HD2	1:A:227:ALA:O	2.20	0.41
1:A:27:PHE:CZ	1:A:174[B]:LEU:CD2	3.03	0.41
1:A:318[B]:LEU:C	1:A:318[B]:LEU:HD13	2.41	0.41
1:A:248:ASP:HB2	1:A:418:LYS:HA	2.02	0.41
1:A:53[B]:ILE:CD1	1:A:179:LEU:HD23	2.48	0.41
2:A:1474:MPD:CM	4:A:2253:HOH:O	2.64	0.41
1:A:301:MET:HB3	1:A:302:ALA:HA	2.01	0.41
1:A:138[A]:LEU:HD23	1:A:138[A]:LEU:HA	1.89	0.41
1:A:305:MET:HE2	1:A:305:MET:HB3	1.82	0.41
1:A:311[A]:ARG:HG2	4:A:2370:HOH:O	2.20	0.41
1:A:82[A]:LEU:HD13	1:A:96:TRP:HH2	1.85	0.41
1:A:161:ASP:OD1	1:A:221[B]:ARG:NH2	2.54	0.41
1:A:298[A]:MET:HB2	1:A:301:MET:HE2	2.03	0.41
1:A:296:MET:O	1:A:302:ALA:HA	2.21	0.40
1:A:380:VAL:CG1	1:A:432[B]:LEU:HD21	2.49	0.40
1:A:278[A]:GLU:HG2	1:A:321:PRO:O	2.21	0.40
1:A:43:LYS:HZ2	1:A:43:LYS:HG2	1.70	0.40
1:A:189:HIS:CA	2:A:1474:MPD:HM1	2.50	0.40
1:A:351[B]:THR:HG22	1:A:352[B]:GLU: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)
4:A:2326:HOH:O	4:A:2388:HOH:O[4_545]	2.17	0.03

## 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	509/439 (116%)	497 (98%)	9 (2%)	3 (1%)	25 11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	MET
1	A	399[A]	VAL
1	A	399[B]	VAL

### 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	439/367 (120%)	428 (98%)	11 (2%)	47	29

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53[A]	ILE
1	A	53[B]	ILE
1	A	53[C]	ILE
1	A	221[A]	ARG
1	A	221[B]	ARG
1	A	303	HIS
1	A	318[A]	LEU
1	A	318[B]	LEU
1	A	323[A]	ASN
1	A	323[B]	ASN
1	A	412	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	137	HIS
1	A	229	ASN
1	A	303	HIS
1	A	388	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 ⓘ

16 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	$\# Z  > 2$
2	MPD	A	1475	-	7,7,7	0.62	0	9,10,10	1.43	1 (11%)
3	MRD	A	1469	-	7,7,7	0.64	0	9,10,10	0.93	1 (11%)
3	MRD	A	1466	-	7,7,7	1.00	0	9,10,10	1.21	1 (11%)
2	MPD	A	1471	-	7,7,7	0.69	0	9,10,10	1.26	1 (11%)
2	MPD	A	1465	-	7,7,7	0.78	0	9,10,10	1.75	2 (22%)
3	MRD	A	1468	-	7,7,7	0.49	0	9,10,10	0.41	0
3	MRD	A	1473	-	7,7,7	0.63	0	9,10,10	0.59	0
2	MPD	A	1463	-	7,7,7	0.33	0	9,10,10	0.31	0
2	MPD	A	1472	-	7,7,7	0.33	0	9,10,10	0.89	0
2	MPD	A	1467	-	7,7,7	0.28	0	9,10,10	0.30	0
3	MRD	A	1476	-	7,7,7	1.00	0	9,10,10	1.97	3 (33%)
3	MRD	A	1464	-	7,7,7	1.09	1 (14%)	9,10,10	0.57	0
2	MPD	A	1474	-	7,7,7	2.95	5 (71%)	9,10,10	6.41	6 (66%)
3	MRD	A	1477	-	7,7,7	2.11	3 (42%)	9,10,10	3.26	4 (44%)
2	MPD	A	1470	-	7,7,7	2.06	3 (42%)	9,10,10	2.68	6 (66%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MPD	A	1478	-	7,7,7	0.54	0	9,10,10	1.11	1 (11%)

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	MPD	A	1475	-	-	2/5/5/5	-
3	MRD	A	1476	-	1/1/2/2	4/5/5/5	-
3	MRD	A	1466	-	-	0/5/5/5	-
2	MPD	A	1471	-	-	1/5/5/5	-
2	MPD	A	1465	-	-	0/5/5/5	-
3	MRD	A	1468	-	-	0/5/5/5	-
3	MRD	A	1469	-	-	0/5/5/5	-
2	MPD	A	1463	-	-	0/5/5/5	-
3	MRD	A	1473	-	-	2/5/5/5	-
2	MPD	A	1472	-	-	2/5/5/5	-
2	MPD	A	1467	-	-	2/5/5/5	-
3	MRD	A	1464	-	-	0/5/5/5	-
2	MPD	A	1474	-	1/1/2/2	2/5/5/5	-
3	MRD	A	1477	-	-	2/5/5/5	-
2	MPD	A	1470	-	-	3/5/5/5	-
2	MPD	A	1478	-	-	0/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1474	MPD	C5-C4	-4.11	1.33	1.51
2	A	1474	MPD	O4-C4	3.95	1.60	1.43
2	A	1470	MPD	O2-C2	3.74	1.54	1.44
3	A	1477	MRD	CM-C2	-3.68	1.41	1.52
3	A	1477	MRD	O2-C2	3.23	1.52	1.44
2	A	1474	MPD	C3-C4	-3.18	1.33	1.51
2	A	1470	MPD	C3-C2	2.59	1.60	1.53
2	A	1474	MPD	O2-C2	-2.54	1.38	1.44
2	A	1474	MPD	CM-C2	-2.43	1.44	1.52
2	A	1470	MPD	C1-C2	-2.41	1.44	1.52
3	A	1477	MRD	C3-C2	-2.25	1.47	1.53
3	A	1464	MRD	O2-C2	-2.13	1.39	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1474	MPD	CM-C2-C1	-10.96	87.73	110.57
2	A	1474	MPD	O2-C2-CM	9.38	138.17	108.08
2	A	1474	MPD	O4-C4-C3	9.33	149.05	111.36
2	A	1474	MPD	O2-C2-C3	-6.76	84.39	109.80
3	A	1477	MRD	CM-C2-C1	-5.37	99.38	110.57
3	A	1477	MRD	O4-C4-C3	-4.86	91.75	111.36
3	A	1477	MRD	O2-C2-C1	4.68	123.08	108.08
2	A	1465	MPD	CM-C2-C1	-4.50	101.20	110.57
2	A	1470	MPD	O2-C2-CM	-4.24	94.48	108.08
2	A	1474	MPD	C1-C2-C3	4.18	129.42	109.96
3	A	1477	MRD	CM-C2-C3	-3.90	91.82	109.96
2	A	1470	MPD	CM-C2-C3	3.72	127.27	109.96
3	A	1476	MRD	CM-C2-C1	-3.58	103.12	110.57
3	A	1476	MRD	O4-C4-C3	3.42	125.19	111.36
2	A	1470	MPD	O4-C4-C5	3.15	123.03	109.38
2	A	1474	MPD	O4-C4-C5	-3.09	96.01	109.38
3	A	1476	MRD	O4-C4-C5	2.85	121.71	109.38
2	A	1475	MPD	O2-C2-C1	-2.41	100.35	108.08
2	A	1470	MPD	C5-C4-C3	-2.37	100.52	111.69
2	A	1470	MPD	O4-C4-C3	2.33	120.78	111.36
2	A	1470	MPD	C1-C2-C3	-2.30	99.23	109.96
2	A	1465	MPD	C1-C2-C3	2.29	120.61	109.96
3	A	1469	MRD	CM-C2-C1	-2.28	105.82	110.57
2	A	1471	MPD	O4-C4-C3	2.25	120.44	111.36
3	A	1466	MRD	O2-C2-C1	2.08	114.74	108.08
2	A	1478	MPD	C1-C2-C3	2.02	119.37	109.96

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1476	MRD	C4
2	A	1474	MPD	C4

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1476	MRD	C1-C2-C3-C4
3	A	1476	MRD	O2-C2-C3-C4
3	A	1476	MRD	C2-C3-C4-C5
3	A	1477	MRD	O2-C2-C3-C4
2	A	1470	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	1467	MPD	C2-C3-C4-C5
2	A	1474	MPD	C2-C3-C4-C5
3	A	1477	MRD	C2-C3-C4-C5
2	A	1470	MPD	C2-C3-C4-C5
3	A	1473	MRD	C2-C3-C4-O4
2	A	1467	MPD	C2-C3-C4-O4
2	A	1472	MPD	C1-C2-C3-C4
3	A	1476	MRD	CM-C2-C3-C4
2	A	1475	MPD	O2-C2-C3-C4
2	A	1471	MPD	C2-C3-C4-C5
3	A	1473	MRD	C2-C3-C4-C5
2	A	1475	MPD	C2-C3-C4-O4
2	A	1472	MPD	C2-C3-C4-O4
2	A	1474	MPD	C2-C3-C4-O4
2	A	1470	MPD	C2-C3-C4-O4

There are no ring outliers.

12 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1475	MPD	20	0
3	A	1469	MRD	2	0
3	A	1466	MRD	3	0
2	A	1471	MPD	3	0
3	A	1468	MRD	5	0
3	A	1473	MRD	3	0
2	A	1472	MPD	1	0
3	A	1476	MRD	12	0
2	A	1474	MPD	23	0
3	A	1477	MRD	4	0
2	A	1470	MPD	1	0
2	A	1478	MPD	9	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 [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	439/439 (100%)	-0.17	12 (2%) 54 58	8, 14, 31, 76	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	MET	7.6
1	A	302	ALA	4.1
1	A	303	HIS	3.9
1	A	300	GLY	3.7
1	A	323[A]	ASN	3.2
1	A	322	LYS	2.9
1	A	338	THR	2.7
1	A	299	GLY	2.5
1	A	410[A]	ARG	2.4
1	A	369	ARG	2.2
1	A	24	GLY	2.1
1	A	26[A]	SER	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MPD	A	1472	8/8	0.64	0.25	30,43,59,66	8
3	MRD	A	1476	8/8	0.66	0.39	16,40,50,51	0
2	MPD	A	1478	8/8	0.70	0.46	39,50,57,78	0
2	MPD	A	1475	8/8	0.72	0.39	19,24,48,49	8
2	MPD	A	1474	8/8	0.77	0.38	28,36,42,55	0
2	MPD	A	1467	8/8	0.85	0.18	23,25,29,31	8
3	MRD	A	1473	8/8	0.85	0.26	37,44,67,68	0
3	MRD	A	1468	8/8	0.85	0.15	24,31,39,47	8
3	MRD	A	1477	8/8	0.88	0.13	33,44,51,53	0
3	MRD	A	1469	8/8	0.89	0.21	21,37,49,53	0
2	MPD	A	1465	8/8	0.90	0.14	26,37,42,50	0
2	MPD	A	1470	8/8	0.90	0.14	26,33,47,48	0
3	MRD	A	1466	8/8	0.92	0.12	33,39,42,43	0
2	MPD	A	1463	8/8	0.92	0.10	12,16,20,21	0
2	MPD	A	1471	8/8	0.92	0.16	23,40,59,64	0
3	MRD	A	1464	8/8	0.95	0.10	17,23,25,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.