



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:21 PM UTC

PDB ID : 4OFZ / pdb_00004ofz
Title : Structure of unliganded trehalose-6-phosphate phosphatase from *Brugia malayi*
Authors : Farelli, J.D.; Allen, K.N.; Carlow, C.K.S.; Dunaway-Mariano, D.
Deposited on : 2014-01-15
Resolution : 3.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

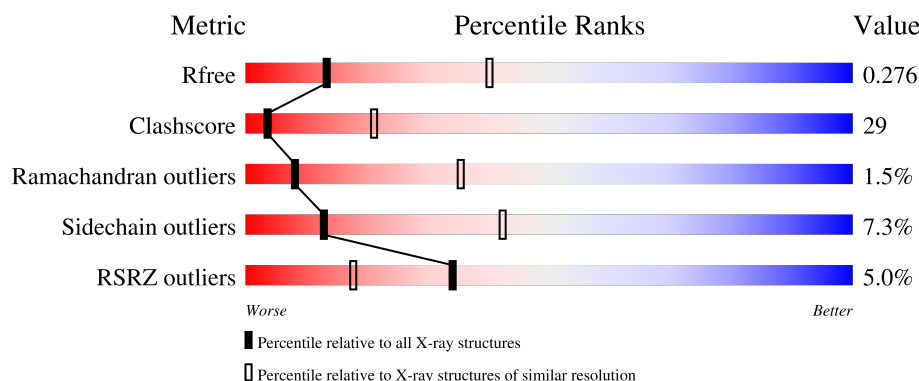
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3384 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 Trehalose-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3296	2084	567	622	23			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A8NS89
A	-20	GLY	-	expression tag	UNP A8NS89
A	-19	SER	-	expression tag	UNP A8NS89
A	-18	SER	-	expression tag	UNP A8NS89
A	-17	HIS	-	expression tag	UNP A8NS89
A	-16	HIS	-	expression tag	UNP A8NS89
A	-15	HIS	-	expression tag	UNP A8NS89
A	-14	HIS	-	expression tag	UNP A8NS89
A	-13	HIS	-	expression tag	UNP A8NS89
A	-12	HIS	-	expression tag	UNP A8NS89
A	-11	SER	-	expression tag	UNP A8NS89
A	-10	SER	-	expression tag	UNP A8NS89
A	-9	GLY	-	expression tag	UNP A8NS89
A	-8	GLY	-	expression tag	UNP A8NS89
A	-7	GLU	-	expression tag	UNP A8NS89
A	-6	ASN	-	expression tag	UNP A8NS89
A	-5	LEU	-	expression tag	UNP A8NS89
A	-4	TYR	-	expression tag	UNP A8NS89
A	-3	PHE	-	expression tag	UNP A8NS89
A	-2	GLN	-	expression tag	UNP A8NS89
A	-1	GLY	-	expression tag	UNP A8NS89
A	0	HIS	-	expression tag	UNP A8NS89

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		

4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.94Å 166.94Å 99.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.91 – 3.00 19.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.91-3.00) 94.4 (19.91-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.216 , 0.273 0.222 , 0.276	Depositor DCC
R_{free} test set	1858 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3384	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.75	4/3353 (0.1%)	1.24	23/4525 (0.5%)

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	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	THR	CA-CB	-6.39	1.37	1.54
1	A	197	PHE	CA-C	6.04	1.60	1.52
1	A	197	PHE	C-O	5.87	1.30	1.24
1	A	198	ILE	C-O	5.77	1.30	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	HIS	CA-C-N	15.40	136.68	120.04
1	A	176	HIS	C-N-CA	15.40	136.68	120.04
1	A	297	ILE	N-CA-C	-12.01	93.57	109.30
1	A	179	GLY	N-CA-C	-8.11	98.87	110.88
1	A	411	ASP	N-CA-C	7.98	120.51	109.18
1	A	441	ASP	N-CA-C	7.68	121.15	111.24
1	A	297	ILE	CA-C-N	7.32	134.87	121.70
1	A	297	ILE	C-N-CA	7.32	134.87	121.70
1	A	298	THR	CA-CB-CG2	-7.15	98.34	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	SER	CA-C-N	-7.14	110.15	120.29
1	A	200	SER	C-N-CA	-7.14	110.15	120.29
1	A	121	THR	CB-CA-C	-6.75	102.31	114.52
1	A	313	LYS	N-CA-C	-6.65	104.03	111.28
1	A	348	HIS	N-CA-C	-6.63	99.66	108.34
1	A	464	ASP	CA-C-N	6.28	133.00	121.70
1	A	464	ASP	C-N-CA	6.28	133.00	121.70
1	A	302	PHE	N-CA-C	-6.22	104.42	111.14
1	A	175	TYR	CB-CA-C	-6.18	100.79	111.30
1	A	301	GLY	N-CA-C	-5.85	105.63	115.80
1	A	393	GLY	N-CA-C	5.83	119.01	110.38
1	A	394	ILE	N-CA-C	-5.58	107.30	112.83
1	A	175	TYR	N-CA-C	5.54	117.75	107.99
1	A	450	ALA	N-CA-C	5.51	118.04	109.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	GLN	Peptide
1	A	258	ARG	Peptide
1	A	298	THR	Peptide
1	A	325	ALA	Peptide
1	A	449	GLY	Peptide

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	3296	0	3316	194	0
2	A	1	0	0	0	0
3	A	87	0	0	26	0
All	All	3384	0	3316	194	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 29.

All (194) 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:390:HIS:CD2	1:A:391:ASN:HA	2.03	0.94
1:A:176:HIS:HB2	1:A:177:PRO:HD3	1.53	0.90
1:A:257:LEU:O	3:A:667:HOH:O	1.90	0.88
1:A:300:GLU:HG2	1:A:301:GLY:N	1.89	0.86
1:A:390:HIS:HA	1:A:391:ASN:C	2.02	0.83
1:A:421:ILE:HG21	3:A:670:HOH:O	1.79	0.82
1:A:398:LYS:NZ	1:A:428:ASP:OD1	2.15	0.76
1:A:153:GLU:N	1:A:153:GLU:OE1	2.19	0.76
1:A:154:GLU:OE2	1:A:154:GLU:N	2.19	0.76
1:A:298:THR:OG1	1:A:299:ASP:N	2.09	0.75
1:A:436:VAL:HG11	1:A:462:ILE:HG22	1.69	0.74
1:A:280:TRP:HE3	1:A:398:LYS:HG3	1.54	0.73
1:A:282:ARG:NH1	1:A:294:GLN:O	2.22	0.73
1:A:176:HIS:HB2	1:A:177:PRO:CD	2.18	0.73
1:A:301:GLY:O	1:A:305:LEU:HG	1.90	0.72
1:A:82:ILE:HD11	1:A:96:ASP:HB3	1.71	0.71
1:A:132:ASP:OD2	1:A:219:LYS:NZ	2.24	0.70
1:A:392:SER:O	3:A:631:HOH:O	2.08	0.70
1:A:298:THR:OG1	1:A:300:GLU:N	2.18	0.70
1:A:392:SER:OG	1:A:393:GLY:N	2.26	0.68
1:A:197:PHE:O	1:A:200:SER:HB3	1.93	0.68
1:A:300:GLU:OE2	1:A:374:ILE:HD13	1.93	0.68
1:A:301:GLY:HA2	1:A:304:ALA:HB3	1.75	0.68
1:A:117:ARG:N	1:A:117:ARG:HD2	2.08	0.68
1:A:223:SER:HB2	1:A:224:GLN:NE2	2.10	0.67
1:A:262:ILE:N	3:A:667:HOH:O	2.26	0.67
1:A:425:THR:O	3:A:671:HOH:O	2.12	0.67
1:A:297:ILE:O	1:A:392:SER:N	2.28	0.66
1:A:467:ARG:O	3:A:643:HOH:O	2.13	0.66
1:A:297:ILE:H	1:A:392:SER:HB3	1.61	0.65
1:A:491:GLY:O	3:A:605:HOH:O	2.14	0.65
1:A:301:GLY:HA3	1:A:374:ILE:HD11	1.79	0.64
1:A:379:PRO:HA	1:A:385:VAL:HG23	1.78	0.64
1:A:298:THR:HG21	1:A:301:GLY:H	1.61	0.64
1:A:238:MET:HB3	3:A:659:HOH:O	1.98	0.64
1:A:338:LEU:N	3:A:651:HOH:O	2.29	0.64
1:A:310:ASP:O	1:A:313:LYS:HG3	1.99	0.63
1:A:483:GLN:NE2	1:A:487:GLU:OE2	2.32	0.62
1:A:120:CYS:HB3	1:A:125:LYS:HG2	1.81	0.62
1:A:269:PRO:O	1:A:270:ILE:HB	2.00	0.62
1:A:115:PHE:O	1:A:117:ARG:NE	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:HG3	1:A:333:ARG:HH11	1.67	0.60
1:A:68:PHE:CE2	1:A:227:THR:HG21	2.37	0.60
1:A:280:TRP:CZ3	1:A:427:SER:HB3	2.37	0.60
1:A:173:ALA:C	1:A:176:HIS:HE1	2.10	0.59
1:A:153:GLU:HA	1:A:155:PRO:HD3	1.84	0.59
1:A:280:TRP:CE3	1:A:398:LYS:HG3	2.36	0.59
1:A:361:VAL:HG12	3:A:634:HOH:O	2.03	0.58
1:A:158:LEU:HB2	1:A:161:ILE:HD12	1.85	0.58
1:A:257:LEU:HD12	1:A:290:ARG:HG3	1.84	0.58
1:A:275:MET:HE1	1:A:409:LEU:HD21	1.86	0.57
1:A:426:LEU:HD12	1:A:429:ILE:HD12	1.86	0.57
1:A:462:ILE:HD11	1:A:468:CYS:SG	2.43	0.57
1:A:445:ALA:N	3:A:643:HOH:O	2.37	0.56
1:A:207:LYS:O	1:A:247:ARG:HD3	2.05	0.56
1:A:110:ASN:N	1:A:110:ASN:OD1	2.39	0.56
1:A:432:VAL:N	3:A:670:HOH:O	2.39	0.56
1:A:124:THR:OG1	1:A:319:SER:OG	2.22	0.56
1:A:319:SER:HA	1:A:323:PRO:HA	1.86	0.55
1:A:223:SER:HB2	1:A:224:GLN:HE21	1.71	0.55
1:A:210:PHE:HD1	1:A:420:LEU:HD23	1.71	0.55
1:A:464:ASP:HA	1:A:465:GLU:CB	2.36	0.55
1:A:365:MET:HG3	1:A:375:LEU:HD11	1.88	0.55
1:A:310:ASP:HA	1:A:313:LYS:HG2	1.89	0.55
1:A:339:THR:HG22	1:A:386:GLU:HG2	1.90	0.54
1:A:210:PHE:CD1	1:A:420:LEU:HD23	2.42	0.54
1:A:311:GLU:HB3	1:A:364:ARG:HD2	1.89	0.54
1:A:116:GLN:NE2	3:A:675:HOH:O	2.22	0.54
1:A:176:HIS:CB	1:A:177:PRO:HD3	2.23	0.54
1:A:440:PRO:O	1:A:467:ARG:NH2	2.41	0.54
1:A:300:GLU:HG3	1:A:374:ILE:HG21	1.90	0.53
1:A:391:ASN:OD1	1:A:391:ASN:N	2.39	0.53
1:A:106:LYS:O	1:A:106:LYS:HD2	2.09	0.53
1:A:213:ASP:OD2	1:A:398:LYS:NZ	2.33	0.53
1:A:377:PHE:CZ	1:A:385:VAL:HG21	2.44	0.53
1:A:121:THR:HG1	1:A:324:PHE:HE1	1.56	0.53
1:A:277:SER:HB3	1:A:284:TRP:CE3	2.43	0.52
1:A:154:GLU:HB3	3:A:641:HOH:O	2.10	0.52
1:A:464:ASP:OD2	1:A:466:SER:OG	2.27	0.52
1:A:214:TRP:HB2	1:A:253:THR:HG22	1.92	0.52
1:A:451:LYS:HG2	1:A:452:MET:H	1.74	0.52
1:A:234:SER:HB2	1:A:478:HIS:CE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE1	1:A:133:GLU:N	2.29	0.51
1:A:256:PRO:HB3	1:A:333:ARG:O	2.09	0.51
1:A:464:ASP:HA	1:A:465:GLU:HB2	1.93	0.51
1:A:123:THR:HG23	1:A:124:THR:HG23	1.93	0.51
1:A:429:ILE:HG12	3:A:655:HOH:O	2.10	0.51
1:A:274:VAL:HG21	3:A:659:HOH:O	2.10	0.51
1:A:78:THR:O	1:A:82:ILE:HD12	2.12	0.50
1:A:302:PHE:HE1	1:A:335:VAL:HG13	1.77	0.50
1:A:297:ILE:N	1:A:392:SER:HB3	2.25	0.50
1:A:298:THR:CB	1:A:300:GLU:H	2.22	0.50
1:A:315:LEU:HD11	1:A:360:ALA:HB1	1.93	0.50
1:A:485:LEU:O	1:A:489:CYS:HB2	2.11	0.50
1:A:422:CYS:HA	1:A:446:ILE:O	2.12	0.49
1:A:239:THR:HG21	1:A:269:PRO:HG2	1.94	0.49
1:A:258:ARG:HG3	1:A:263:LEU:HD22	1.94	0.49
1:A:197:PHE:HZ	3:A:677:HOH:O	1.95	0.49
1:A:297:ILE:HB	1:A:391:ASN:HB3	1.93	0.49
1:A:300:GLU:HG3	1:A:374:ILE:HG12	1.95	0.49
1:A:307:ARG:O	1:A:310:ASP:HB2	2.12	0.49
1:A:79:ARG:CZ	1:A:231:PRO:HA	2.43	0.48
1:A:398:LYS:HB3	1:A:431:MET:HG3	1.94	0.48
1:A:211:ILE:O	3:A:652:HOH:O	2.20	0.48
1:A:297:ILE:CG1	1:A:392:SER:HB2	2.44	0.48
1:A:331:VAL:HB	1:A:340:LEU:HD21	1.94	0.48
1:A:301:GLY:HA2	1:A:304:ALA:CB	2.42	0.48
1:A:242:ALA:HB1	3:A:615:HOH:O	2.14	0.48
1:A:261:GLY:O	1:A:265:LEU:HG	2.13	0.48
1:A:235:ALA:O	1:A:239:THR:OG1	2.26	0.48
1:A:310:ASP:O	1:A:313:LYS:N	2.46	0.47
1:A:175:TYR:O	1:A:176:HIS:HB3	2.13	0.47
1:A:200:SER:HB2	1:A:418:LYS:HG3	1.96	0.47
1:A:297:ILE:O	1:A:391:ASN:C	2.58	0.47
1:A:79:ARG:HG2	1:A:232:VAL:HG23	1.96	0.47
1:A:254:ALA:O	1:A:334:LYS:HE2	2.13	0.47
1:A:451:LYS:HG2	1:A:452:MET:N	2.30	0.47
1:A:259:GLY:HA2	1:A:260:PRO:HA	1.59	0.47
1:A:390:HIS:CD2	1:A:391:ASN:CA	2.90	0.47
1:A:72:MET:HE3	1:A:229:LEU:HD12	1.97	0.47
1:A:343:GLN:HA	1:A:349:VAL:HG11	1.96	0.47
1:A:246:THR:HB	3:A:677:HOH:O	2.14	0.46
1:A:297:ILE:HD12	1:A:392:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ARG:HA	1:A:105:GLU:HG2	1.97	0.46
1:A:278:GLY:HA3	3:A:682:HOH:O	2.14	0.46
1:A:177:PRO:HD2	1:A:178:LYS:HG3	1.96	0.46
1:A:316:LEU:HD11	1:A:331:VAL:HG11	1.97	0.46
1:A:280:TRP:HZ3	1:A:427:SER:HB3	1.80	0.46
1:A:75:MET:HE2	1:A:79:ARG:HD2	1.98	0.46
1:A:235:ALA:HB2	1:A:267:ALA:HB3	1.98	0.46
1:A:413:LEU:HD22	1:A:419:ILE:HD13	1.98	0.46
1:A:177:PRO:HD2	1:A:178:LYS:CG	2.45	0.46
1:A:106:LYS:HD2	1:A:106:LYS:C	2.41	0.45
1:A:448:VAL:HG22	1:A:471:VAL:HG23	1.98	0.45
1:A:263:LEU:N	3:A:667:HOH:O	2.02	0.45
1:A:281:GLY:HA3	1:A:401:GLY:HA3	1.97	0.45
1:A:306:GLN:OE1	1:A:333:ARG:NE	2.39	0.45
1:A:219:LYS:HE3	1:A:228:ASN:OD1	2.16	0.45
1:A:300:GLU:CG	1:A:301:GLY:N	2.70	0.45
1:A:110:ASN:O	1:A:117:ARG:NH2	2.48	0.45
1:A:196:THR:O	1:A:199:SER:OG	2.25	0.44
1:A:343:GLN:HB3	1:A:383:LEU:HA	1.98	0.44
1:A:300:GLU:HG2	1:A:301:GLY:H	1.80	0.44
1:A:168:LEU:N	3:A:660:HOH:O	2.50	0.44
1:A:298:THR:H	1:A:298:THR:HG22	1.26	0.44
1:A:439:ASN:O	1:A:443:VAL:HG23	2.18	0.44
1:A:391:ASN:HA	1:A:392:SER:HA	1.78	0.44
1:A:200:SER:HB2	1:A:418:LYS:CG	2.48	0.44
1:A:360:ALA:O	1:A:364:ARG:HG2	2.17	0.44
1:A:365:MET:HE2	1:A:387:VAL:HG13	2.00	0.44
1:A:191:VAL:HG13	1:A:484:ILE:HD11	2.00	0.44
1:A:75:MET:HG3	1:A:100:LEU:CD2	2.48	0.44
1:A:194:LEU:O	1:A:198:ILE:HG12	2.18	0.44
1:A:298:THR:OG1	1:A:300:GLU:HB3	2.18	0.44
1:A:228:ASN:HB3	1:A:265:LEU:HD13	2.00	0.43
1:A:315:LEU:HD12	1:A:364:ARG:HE	1.82	0.43
1:A:283:GLU:HB3	1:A:292:VAL:HG22	1.99	0.43
1:A:362:LYS:HG2	3:A:634:HOH:O	2.18	0.43
1:A:280:TRP:CH2	1:A:427:SER:HB3	2.53	0.43
1:A:94:LYS:HE2	1:A:148:MET:HE1	2.01	0.43
1:A:79:ARG:HG2	1:A:232:VAL:CG2	2.49	0.43
1:A:176:HIS:CB	1:A:177:PRO:CD	2.90	0.42
1:A:121:THR:HG21	1:A:319:SER:HB2	2.02	0.42
1:A:159:TRP:HB2	1:A:160:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:THR:O	1:A:352:GLU:N	2.53	0.42
1:A:452:MET:HE3	1:A:452:MET:HB2	1.88	0.42
1:A:390:HIS:CD2	1:A:392:SER:HA	2.55	0.42
1:A:421:ILE:HD13	3:A:670:HOH:O	2.20	0.42
1:A:366:HIS:CD2	1:A:373:GLN:H	2.37	0.41
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.80	0.41
1:A:298:THR:HG21	1:A:300:GLU:CD	2.46	0.41
1:A:327:VAL:O	1:A:328:GLY:C	2.63	0.41
1:A:457:GLU:OE1	1:A:457:GLU:HA	2.20	0.41
1:A:230:GLN:HA	1:A:231:PRO:HD2	1.95	0.41
1:A:347:HIS:O	1:A:348:HIS:ND1	2.51	0.41
1:A:365:MET:HE3	3:A:634:HOH:O	2.21	0.41
1:A:161:ILE:O	1:A:164:SER:OG	2.31	0.41
1:A:297:ILE:O	1:A:391:ASN:O	2.38	0.41
1:A:484:ILE:HD13	1:A:484:ILE:HA	1.89	0.41
1:A:186:GLU:O	1:A:190:THR:OG1	2.36	0.41
1:A:333:ARG:NH1	1:A:334:LYS:O	2.54	0.41
1:A:240:ARG:O	1:A:244:SER:OG	2.34	0.40
1:A:116:GLN:N	1:A:116:GLN:CD	2.79	0.40
1:A:129:ASN:O	1:A:224:GLN:NE2	2.42	0.40
1:A:154:GLU:HA	1:A:155:PRO:HD3	1.86	0.40
1:A:375:LEU:HD13	1:A:387:VAL:CG1	2.51	0.40
1:A:151:ARG:NH1	1:A:157:LEU:O	2.54	0.40
1:A:227:THR:O	1:A:229:LEU:HG	2.21	0.40
1:A:374:ILE:HD12	1:A:375:LEU:N	2.36	0.40
1:A:439:ASN:OD1	1:A:442:GLY:HA3	2.21	0.40
1:A:173:ALA:C	1:A:176:HIS:CE1	2.97	0.40
1:A:398:LYS:HB3	1:A:431:MET:CG	2.52	0.40
1:A:448:VAL:HG22	1:A:471:VAL:CG2	2.52	0.40
1:A:464:ASP:HB2	1:A:466:SER:H	1.86	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	410/514 (80%)	379 (92%)	25 (6%)	6 (2%)	8	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
1	A	326	LEU
1	A	327	VAL
1	A	331	VAL
1	A	395	ILE
1	A	260	PRO

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	368/451 (82%)	341 (93%)	27 (7%)	13	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	MET
1	A	82	ILE
1	A	93	THR
1	A	95	ASP
1	A	110	ASN
1	A	117	ARG
1	A	121	THR
1	A	126	LEU
1	A	130	ILE
1	A	178	LYS
1	A	244	SER
1	A	246	THR
1	A	247	ARG

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Mol	Chain	Res	Type
1	A	289	LYS
1	A	291	VAL
1	A	299	ASP
1	A	300	GLU
1	A	340	LEU
1	A	344	THR
1	A	345	VAL
1	A	374	ILE
1	A	383	LEU
1	A	394	ILE
1	A	414	GLN
1	A	453	SER
1	A	472	SER
1	A	490	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	176	HIS
1	A	294	GLN
1	A	390	HIS
1	A	438	GLN
1	A	460	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/514 (81%)	-0.04	21 (5%) 34 18	34, 68, 130, 258	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ILE	6.5
1	A	324	PHE	6.5
1	A	300	GLU	5.8
1	A	287	SER	4.2
1	A	280	TRP	3.9
1	A	442	GLY	3.4
1	A	371	ASN	3.3
1	A	115	PHE	3.2
1	A	366	HIS	3.2
1	A	177	PRO	3.2
1	A	327	VAL	3.1
1	A	176	HIS	3.0
1	A	178	LYS	2.9
1	A	116	GLN	2.6
1	A	296	GLY	2.6
1	A	328	GLY	2.5
1	A	449	GLY	2.2
1	A	357	TYR	2.1
1	A	259	GLY	2.1
1	A	373	GLN	2.1
1	A	323	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	501	1/1	0.84	0.10	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.