



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:40 PM GMT

PDB ID : 1Q50  
Title : Phosphoglucose isomerase from *Leishmania mexicana*.  
Authors : Cordeiro, A.T.; Michels, P.A.M.; Delboni, L.F.; Thiemann, O.H.  
Deposited on : 2003-08-05  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

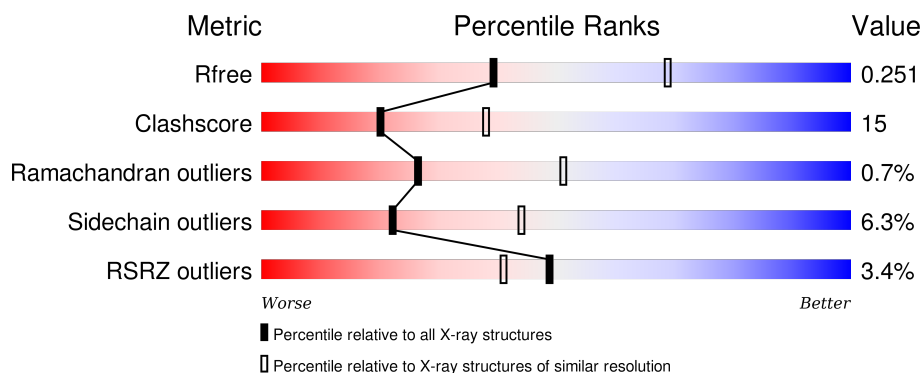
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	561	<div> <div>3%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4603 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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4387	2774	763	828	22			

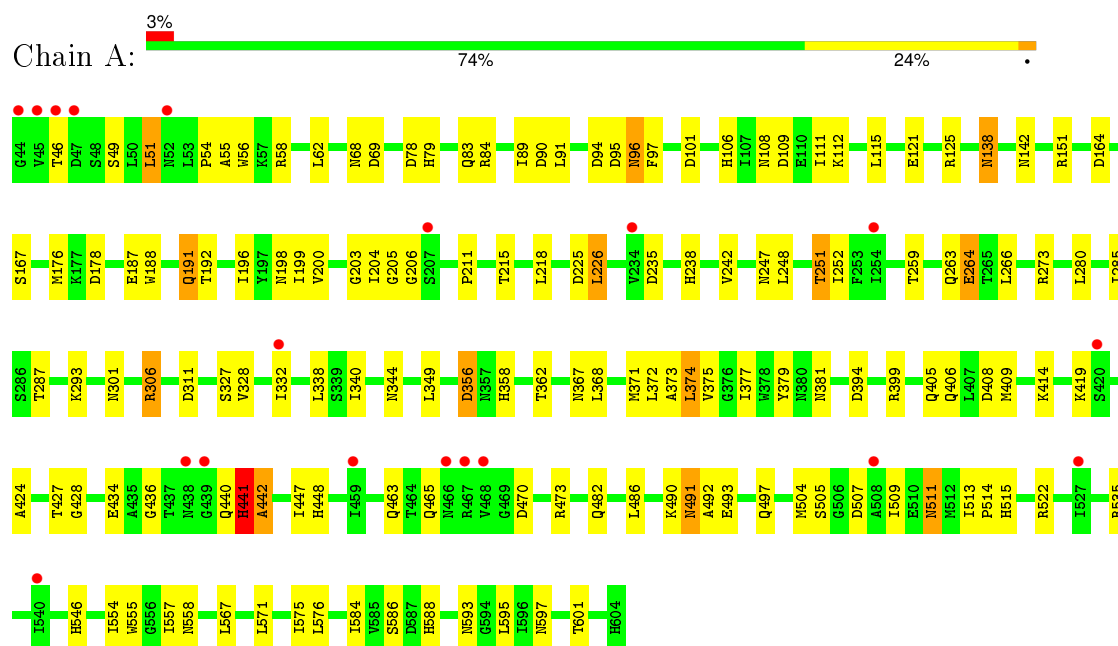
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	216	Total	O	0	0
			216	216		

### 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 ( $\text{RSRZ} > 2$ ). 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: Glucose-6-phosphate isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.74Å 85.74Å 350.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.60) 98.7 (29.28-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.09	Depositor
R, $R_{free}$	0.195 , 0.250 0.209 , 0.251	Depositor DCC
$R_{free}$ test set	1203 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 31.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43433 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4603	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

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	0.93	3/4479 (0.1%)	1.01	21/6064 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	MET	SD-CE	-5.69	1.46	1.77
1	A	167	SER	CB-OG	-5.65	1.34	1.42
1	A	176	MET	SD-CE	-5.27	1.48	1.77

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASP	CB-CG-OD2	9.06	126.46	118.30
1	A	522	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	394	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	535	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	164	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	90	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	328	VAL	CB-CA-C	-6.52	99.00	111.40
1	A	356	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	522	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	311	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	311	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	A	507	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	178	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	69	ASP	CB-CG-OD2	5.57	123.32	118.30
1	A	225	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	470	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	473	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	101	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	95	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	408	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	306	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4387	0	4302	128	1
2	A	216	0	0	16	0
All	All	4603	0	4302	128	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 15.

All (128) 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:203:GLY:O	1:A:204:ILE:HG13	1.44	1.18
1:A:196:ILE:HD13	1:A:252:ILE:CD1	1.75	1.16
1:A:196:ILE:CD1	1:A:252:ILE:HD11	1.81	1.09
1:A:340:ILE:HG22	1:A:344:ASN:HB2	1.23	1.08
1:A:46:THR:HG21	2:A:683:HOH:O	1.54	1.07
1:A:327:SER:HB2	1:A:332:ILE:CD1	1.84	1.06
1:A:414:LYS:HB2	1:A:557:ILE:HD13	1.39	1.05
1:A:427:THR:HG21	1:A:557:ILE:HD11	1.38	1.03
1:A:340:ILE:HG22	1:A:344:ASN:CB	1.90	1.01
1:A:327:SER:HB2	1:A:332:ILE:HD12	1.03	1.00
1:A:557:ILE:HG23	2:A:721:HOH:O	1.65	0.97
1:A:196:ILE:HD13	1:A:252:ILE:CG1	1.97	0.95
1:A:327:SER:CB	1:A:332:ILE:HD12	1.96	0.94
1:A:597:ASN:O	1:A:601:THR:HG23	1.69	0.91
1:A:505:SER:O	1:A:509:ILE:HG13	1.72	0.89
1:A:196:ILE:CD1	1:A:252:ILE:CD1	2.44	0.89
1:A:218:LEU:HB2	1:A:340:ILE:HD11	1.54	0.88
1:A:199:ILE:HD13	1:A:338:LEU:HD13	1.54	0.88
1:A:377:ILE:HD11	1:A:554:ILE:HD12	1.57	0.87
1:A:96:ASN:HD22	1:A:97:PHE:H	1.20	0.86
1:A:340:ILE:CG2	1:A:344:ASN:CB	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ILE:HD13	1:A:252:ILE:HG13	1.59	0.81
1:A:188:TRP:CD1	1:A:196:ILE:HD11	2.16	0.80
1:A:142:ASN:ND2	2:A:681:HOH:O	2.16	0.77
1:A:491:ASN:HD22	1:A:492:ALA:H	1.32	0.75
1:A:491:ASN:ND2	1:A:492:ALA:H	1.87	0.72
1:A:79:HIS:HD2	2:A:738:HOH:O	1.73	0.72
1:A:557:ILE:HG22	1:A:558:ASN:N	2.03	0.72
1:A:377:ILE:CD1	1:A:554:ILE:CD1	2.69	0.71
1:A:327:SER:CB	1:A:332:ILE:CD1	2.63	0.70
1:A:96:ASN:HD22	1:A:97:PHE:N	1.90	0.70
1:A:203:GLY:O	1:A:204:ILE:CG1	2.32	0.69
1:A:89:ILE:HG12	1:A:358:HIS:CD2	2.29	0.68
1:A:505:SER:O	1:A:509:ILE:CG1	2.41	0.68
1:A:427:THR:HG21	1:A:557:ILE:CD1	2.21	0.67
1:A:191:GLN:HA	1:A:191:GLN:HE21	1.60	0.67
1:A:340:ILE:CG2	1:A:344:ASN:HB3	2.25	0.67
1:A:441:HIS:O	1:A:442:ALA:C	2.32	0.66
1:A:206:GLY:HA2	1:A:406:GLN:HE22	1.60	0.66
1:A:557:ILE:CG2	1:A:558:ASN:N	2.59	0.66
1:A:601:THR:HG22	2:A:615:HOH:O	1.95	0.65
1:A:340:ILE:HG22	1:A:340:ILE:O	1.96	0.65
1:A:414:LYS:HG3	1:A:557:ILE:HG21	1.80	0.63
1:A:504:MET:HB3	1:A:509:ILE:HG12	1.81	0.62
1:A:203:GLY:C	1:A:204:ILE:HG13	2.18	0.61
1:A:491:ASN:ND2	1:A:492:ALA:N	2.48	0.61
1:A:106:HIS:HD2	1:A:379:TYR:OH	1.84	0.61
1:A:504:MET:O	1:A:509:ILE:HD11	2.01	0.60
1:A:199:ILE:CD1	1:A:338:LEU:HD13	2.29	0.60
1:A:377:ILE:CD1	1:A:554:ILE:HD13	2.31	0.60
1:A:340:ILE:HG21	1:A:344:ASN:HB3	1.83	0.60
1:A:588:HIS:H	1:A:593:ASN:HD21	1.50	0.60
1:A:491:ASN:HD22	1:A:492:ALA:N	1.99	0.59
1:A:125:ARG:NH2	1:A:362:THR:O	2.36	0.59
1:A:218:LEU:CB	1:A:340:ILE:HD11	2.31	0.58
1:A:377:ILE:HD11	1:A:554:ILE:CD1	2.27	0.58
1:A:196:ILE:CD1	1:A:252:ILE:CG1	2.75	0.58
1:A:204:ILE:HG22	1:A:205:GLY:N	2.18	0.57
1:A:490:LYS:CE	2:A:799:HOH:O	2.53	0.57
1:A:358:HIS:CE1	1:A:368:LEU:H	2.23	0.57
1:A:188:TRP:CD1	1:A:196:ILE:CD1	2.86	0.56
1:A:505:SER:O	1:A:509:ILE:CD1	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:HIS:HE1	1:A:368:LEU:H	1.53	0.56
1:A:79:HIS:HB3	2:A:633:HOH:O	2.04	0.56
1:A:125:ARG:HB2	1:A:125:ARG:HH11	1.72	0.55
1:A:434:GLU:OE2	2:A:696:HOH:O	2.18	0.55
1:A:198:ASN:HB2	1:A:251:THR:HB	1.88	0.54
1:A:436:GLY:O	1:A:440:GLN:HB3	2.08	0.54
1:A:204:ILE:HD11	1:A:264:GLU:OE1	2.08	0.54
1:A:441:HIS:ND1	1:A:442:ALA:N	2.56	0.53
1:A:199:ILE:HD13	1:A:338:LEU:CD1	2.35	0.53
1:A:238:HIS:O	1:A:242:VAL:HG12	2.09	0.53
1:A:211:PRO:O	1:A:215:THR:HG23	2.09	0.52
1:A:204:ILE:CG2	1:A:205:GLY:N	2.72	0.52
1:A:377:ILE:HG23	1:A:381:ASN:HD22	1.73	0.52
1:A:448:HIS:HE1	1:A:482:GLN:OE1	1.93	0.52
1:A:196:ILE:CD1	1:A:252:ILE:HG13	2.32	0.52
1:A:493:GLU:O	1:A:497:GLN:HG2	2.09	0.52
1:A:414:LYS:CB	1:A:557:ILE:HG21	2.40	0.52
1:A:58:ARG:O	1:A:62:LEU:HD13	2.09	0.51
1:A:196:ILE:HD12	1:A:252:ILE:HD11	1.83	0.51
1:A:373:ALA:O	1:A:377:ILE:HG13	2.10	0.51
1:A:191:GLN:NE2	1:A:293:LYS:HD2	2.26	0.51
1:A:247:ASN:O	1:A:251:THR:HG22	2.10	0.50
1:A:84:ARG:O	1:A:112:LYS:NZ	2.45	0.50
1:A:340:ILE:CG2	1:A:340:ILE:O	2.60	0.50
1:A:571:LEU:O	1:A:575:ILE:HG13	2.11	0.50
1:A:192:THR:HG22	1:A:285:ILE:HD13	1.93	0.50
1:A:427:THR:CG2	1:A:557:ILE:HD11	2.27	0.49
1:A:356:ASP:OD1	1:A:546:HIS:HE1	1.96	0.49
1:A:377:ILE:HD13	1:A:554:ILE:HD13	1.94	0.49
1:A:381:ASN:HD21	1:A:555:TRP:HE1	1.60	0.49
1:A:358:HIS:HE1	1:A:367:ASN:HA	1.76	0.49
1:A:448:HIS:HD2	2:A:621:HOH:O	1.96	0.49
1:A:414:LYS:CG	1:A:557:ILE:HG21	2.44	0.48
1:A:368:LEU:HD23	1:A:368:LEU:C	2.34	0.48
1:A:515:HIS:HD2	2:A:610:HOH:O	1.96	0.48
1:A:68:ASN:ND2	2:A:776:HOH:O	2.47	0.48
1:A:414:LYS:HB2	1:A:557:ILE:HG21	1.95	0.47
1:A:273:ARG:HD2	2:A:685:HOH:O	2.13	0.47
1:A:187:GLU:O	1:A:187:GLU:HG2	2.15	0.47
1:A:381:ASN:ND2	1:A:555:TRP:HE1	2.12	0.47
1:A:504:MET:HB3	1:A:509:ILE:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HB3	1:A:374:LEU:HG	1.98	0.46
1:A:509:ILE:O	1:A:513:ILE:HG13	2.15	0.46
1:A:191:GLN:HA	1:A:191:GLN:NE2	2.31	0.45
1:A:248:LEU:HA	1:A:251:THR:CG2	2.47	0.45
1:A:84:ARG:NH2	1:A:109:ASP:OD2	2.50	0.45
1:A:490:LYS:HE2	2:A:799:HOH:O	2.16	0.44
1:A:280:LEU:HD23	1:A:287:THR:HA	1.99	0.44
1:A:377:ILE:CD1	1:A:554:ILE:HD12	2.28	0.44
1:A:55:ALA:HB2	1:A:121:GLU:CD	2.38	0.44
1:A:259:THR:O	1:A:301:ASN:ND2	2.47	0.43
1:A:405:GLN:HB3	1:A:409:MET:HE3	2.00	0.43
1:A:199:ILE:HD12	1:A:226:LEU:HD21	2.00	0.43
1:A:196:ILE:HD13	1:A:252:ILE:HD12	1.84	0.43
1:A:447:ILE:HG22	1:A:486:LEU:HD21	2.00	0.42
1:A:51:LEU:HD12	1:A:424:ALA:HB1	2.00	0.42
1:A:428:GLY:HA3	2:A:711:HOH:O	2.19	0.42
1:A:511:ASN:HD22	1:A:511:ASN:C	2.23	0.42
1:A:377:ILE:HG23	1:A:381:ASN:ND2	2.33	0.42
1:A:414:LYS:HG3	1:A:557:ILE:CG2	2.50	0.41
1:A:513:ILE:HB	1:A:514:PRO:HD3	2.02	0.41
1:A:513:ILE:HB	1:A:514:PRO:CD	2.50	0.41
1:A:108:ASN:H	1:A:111:ILE:HD12	1.85	0.41
1:A:79:HIS:CD2	2:A:738:HOH:O	2.58	0.41
1:A:54:PRO:HD2	2:A:754:HOH:O	2.19	0.41
1:A:138:ASN:ND2	1:A:558:ASN:OD1	2.53	0.41

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)
1:A:306:ARG:O	1:A:584:ILE:CD1[9_655]	2.17	0.03

## 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	559/561 (100%)	531 (95%)	24 (4%)	4 (1%)	26	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	LYS
1	A	441	HIS
1	A	442	ALA
1	A	465	GLN

### 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	474/475 (100%)	444 (94%)	30 (6%)	22	44

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	51	LEU
1	A	56	TRP
1	A	78	ASP
1	A	83	GLN
1	A	91	LEU
1	A	94	ASP
1	A	96	ASN
1	A	138	ASN
1	A	151	ARG
1	A	191	GLN
1	A	200	VAL
1	A	226	LEU
1	A	251	THR
1	A	263	GLN

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Mol	Chain	Res	Type
1	A	264	GLU
1	A	266	LEU
1	A	349	LEU
1	A	372	LEU
1	A	374	LEU
1	A	375	VAL
1	A	399	ARG
1	A	441	HIS
1	A	463	GLN
1	A	491	ASN
1	A	511	ASN
1	A	567	LEU
1	A	576	LEU
1	A	586	SER
1	A	595	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	83	GLN
1	A	92	HIS
1	A	96	ASN
1	A	106	HIS
1	A	138	ASN
1	A	142	ASN
1	A	147	HIS
1	A	175	GLN
1	A	191	GLN
1	A	201	ASN
1	A	233	ASN
1	A	263	GLN
1	A	357	ASN
1	A	358	HIS
1	A	380	ASN
1	A	381	ASN
1	A	405	GLN
1	A	406	GLN
1	A	440	GLN
1	A	448	HIS
1	A	463	GLN
1	A	491	ASN

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Mol	Chain	Res	Type
1	A	511	ASN
1	A	546	HIS
1	A	558	ASN
1	A	583	ASN
1	A	593	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](#)

There are no ligands in this entry.

## 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	561/561 (100%)	-0.32	19 (3%) 49 41	15, 30, 65, 82	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	GLY	7.1
1	A	45	VAL	4.7
1	A	439	GLY	4.0
1	A	527	ILE	3.8
1	A	468	VAL	3.6
1	A	207	SER	3.2
1	A	332	ILE	2.8
1	A	459	ILE	2.8
1	A	420	SER	2.7
1	A	254	ILE	2.7
1	A	47	ASP	2.6
1	A	438	ASN	2.5
1	A	46	THR	2.5
1	A	52	ASN	2.3
1	A	540	ILE	2.2
1	A	508	ALA	2.1
1	A	466	ASN	2.1
1	A	467	ARG	2.0
1	A	234	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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.