



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:50 PM GMT

PDB ID : 1HM5  
Title : CRYSTAL STRUCTURE ANALYSIS OF THE RABBIT D-GLUCOSE 6-PHOSPHATE ISOMERASE (NO LIGAND BOUND)  
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Deposited on : 2000-12-04  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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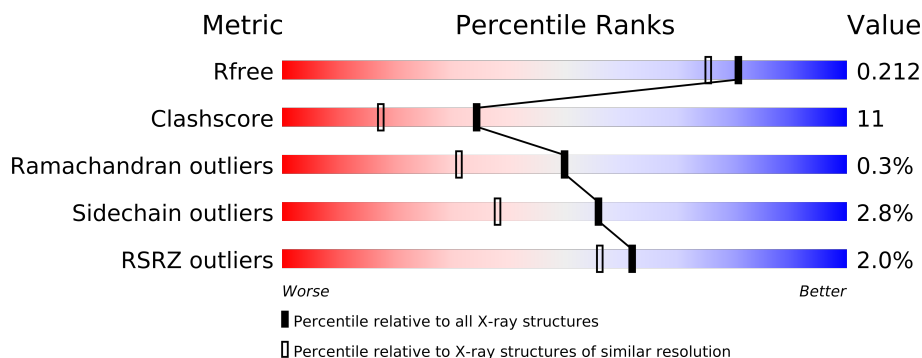
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	558	
1	B	558	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9740 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHOGLUCOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4407	2814	767	807	19			
1	B	556	Total	C	N	O	S	0	0	0
			4407	2814	767	807	19			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	451	Total	O	0	0
			451	451		
2	B	475	Total	O	0	0
			475	475		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.76Å 115.97Å 271.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 39.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.5 (10.00-1.80) 85.4 (39.66-1.80)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.183 , 0.212 0.183 , 0.212	Depositor DCC
$R_{free}$ test set	10314 reflections (10.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105352 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.37	0/4516	0.60	0/6116
1	B	0.40	0/4516	0.64	2/6116 (0.0%)
All	All	0.39	0/9032	0.62	2/12232 (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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	B	384	THR	O-C-N	-5.52	113.87	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	GLY	Mainchain,Peptide
1	B	383	GLY	Mainchain,Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4407	0	4374	105	0
1	B	4407	0	4374	96	0
2	A	451	0	0	11	0
2	B	475	0	0	13	0
All	All	9740	0	8748	190	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (190) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:345:HIS:HA	1:A:382:PRO:HG3	1.49	0.94
1:A:186:ILE:HB	1:A:216:GLU:HG2	1.50	0.93
1:B:537:HIS:H	1:B:542:ASN:HD21	1.24	0.86
1:B:345:HIS:HA	1:B:382:PRO:HG3	1.58	0.84
1:A:445:ARG:HG2	1:A:449:GLN:HE21	1.44	0.83
1:B:156:ILE:HG13	2:B:816:HOH:O	1.77	0.82
1:A:537:HIS:H	1:A:542:ASN:HD21	1.28	0.82
1:A:550:GLN:HE21	1:A:551:GLN:HE21	1.27	0.81
1:B:305:HIS:HE1	1:B:315:ALA:H	1.28	0.81
1:B:550:GLN:HE21	1:B:551:GLN:HE21	1.26	0.80
1:B:6:ASN:HD21	1:B:8:GLN:HB2	1.50	0.77
1:A:2:ALA:O	1:A:5:ARG:HG2	1.88	0.74
1:A:175:SER:HB2	2:A:781:HOH:O	1.86	0.73
1:B:312:GLU:H	1:B:312:GLU:CD	1.91	0.73
1:A:272:ARG:HH12	1:A:511:GLN:HE21	1.36	0.73
1:B:272:ARG:HH12	1:B:511:GLN:HE21	1.35	0.72
1:A:68:LEU:O	1:A:72:LYS:HG3	1.90	0.71
1:A:144:THR:HG21	1:A:201:GLU:OE1	1.91	0.70
1:A:456:GLU:O	1:A:460:LYS:HE2	1.94	0.67
1:B:199:ASN:OD1	1:B:201:GLU:HG2	1.94	0.67
1:B:186:ILE:HB	1:B:216:GLU:HG2	1.77	0.66
1:A:556:ILE:O	1:A:556:ILE:HG22	1.94	0.66
1:B:14:GLN:O	1:B:18:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:384:THR:O	1:B:385:ASN:C	2.32	0.64
1:A:12:LEU:HD11	1:A:67:LEU:HD23	1.80	0.64
1:B:6:ASN:HD22	1:B:9:PHE:H	1.44	0.64
1:B:553:GLU:HB2	2:B:868:HOH:O	1.97	0.63
1:A:272:ARG:HH12	1:A:511:GLN:NE2	1.97	0.62
1:A:129:LYS:O	1:A:133:GLN:HG3	2.00	0.61
1:B:16:HIS:O	1:B:20:GLY:N	2.32	0.61
1:B:210:LYS:HG2	1:B:265:PHE:CE1	2.35	0.61
1:A:369:ARG:HH11	1:A:369:ARG:HG2	1.65	0.60
1:B:395:HIS:HD2	2:B:583:HOH:O	1.83	0.60
1:B:343:TYR:OH	1:B:413:HIS:HE1	1.85	0.60
1:A:2:ALA:HA	1:A:5:ARG:NE	2.17	0.59
1:B:303:ASP:OD1	1:B:495:HIS:HE1	1.84	0.59
1:B:132:CYS:HB3	2:B:799:HOH:O	2.02	0.59
1:A:518:LYS:HB2	1:A:518:LYS:NZ	2.17	0.59
1:B:272:ARG:HH12	1:B:511:GLN:NE2	2.01	0.59
1:A:209:SER:O	1:A:246:SER:HB2	2.02	0.58
1:B:210:LYS:HE2	2:B:936:HOH:O	2.03	0.58
1:B:387:GLN:HA	1:B:391:TYR:CD1	2.39	0.58
1:A:264:GLU:HG2	2:A:721:HOH:O	2.03	0.57
1:B:90:ASN:ND2	1:B:507:ASN:HD21	2.02	0.57
1:A:12:LEU:HD11	1:A:67:LEU:CD2	2.34	0.57
1:B:521:ALA:O	1:B:525:GLU:HG3	2.04	0.57
1:B:156:ILE:HD12	1:B:184:SER:O	2.05	0.57
1:A:223:THR:OG1	1:B:420:HIS:HE1	1.88	0.56
1:B:6:ASN:ND2	1:B:8:GLN:H	2.03	0.56
1:A:41:LEU:HD12	1:A:41:LEU:O	2.05	0.56
1:A:514:VAL:HG12	2:A:828:HOH:O	2.05	0.56
1:A:45:THR:O	1:A:46:ASN:HB2	2.06	0.56
1:B:516:LEU:O	1:B:519:GLN:HG2	2.07	0.55
1:B:14:GLN:O	1:B:17:ARG:HB3	2.05	0.55
1:A:420:HIS:HE1	1:B:223:THR:OG1	1.89	0.55
1:B:395:HIS:HE1	1:B:431:GLN:OE1	1.89	0.55
1:A:90:ASN:ND2	1:A:507:ASN:HD21	2.05	0.55
1:A:303:ASP:OD1	1:A:495:HIS:HE1	1.90	0.55
1:A:136:ARG:HD3	1:A:285:LEU:O	2.06	0.55
1:A:514:VAL:CG1	2:A:828:HOH:O	2.55	0.54
1:A:520:LEU:HD12	1:B:434:ALA:HB2	1.88	0.54
1:B:161:LEU:HD13	1:B:350:TYR:HA	1.90	0.54
1:A:416:ARG:HH12	1:B:222:LYS:NZ	2.05	0.54
1:B:45:THR:O	1:B:46:ASN:HB2	2.08	0.54
1:B:305:HIS:CE1	1:B:315:ALA:H	2.17	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:152:ILE:N	1:A:152:ILE:HD12	2.23	0.53
1:A:74:ARG:NH2	1:A:505:ASP:HB2	2.23	0.53
1:A:387:GLN:HE22	1:A:427:ASN:HB3	1.74	0.53
1:B:16:HIS:HE1	1:B:330:PHE:CZ	2.27	0.53
2:A:604:HOH:O	1:B:49:HIS:HD2	1.91	0.53
1:A:448:LEU:HD11	1:A:465:LYS:HD3	1.92	0.52
1:A:416:ARG:HH12	1:B:222:LYS:HZ3	1.58	0.52
1:B:95:ARG:HD2	2:B:1003:HOH:O	2.09	0.52
1:B:6:ASN:ND2	1:B:8:GLN:HB2	2.21	0.52
1:A:123:LYS:C	1:A:123:LYS:HD3	2.30	0.52
1:A:387:GLN:HA	1:A:391:TYR:CD1	2.45	0.52
1:A:22:GLU:OE1	1:A:23:LEU:N	2.44	0.51
1:B:98:LEU:HB2	1:B:268:TRP:CE3	2.45	0.51
1:A:216:GLU:CD	1:B:388:HIS:HE2	2.13	0.51
1:A:68:LEU:HD13	1:A:312:GLU:HG3	1.92	0.51
2:A:757:HOH:O	1:B:49:HIS:HE1	1.93	0.51
1:A:164:LEU:C	1:A:164:LEU:HD23	2.31	0.51
1:B:518:LYS:HE2	2:B:942:HOH:O	2.11	0.50
1:B:369:ARG:HH11	1:B:369:ARG:HG2	1.75	0.50
1:A:516:LEU:O	1:A:519:GLN:HG2	2.11	0.50
1:B:511:GLN:O	1:B:514:VAL:HG12	2.12	0.50
1:A:382:PRO:O	1:A:385:ASN:HB2	2.12	0.50
1:A:98:LEU:HB2	1:A:268:TRP:CE3	2.47	0.50
1:B:258:ASP:HB3	1:B:261:ASN:ND2	2.27	0.50
1:B:186:ILE:HB	1:B:216:GLU:CG	2.42	0.49
1:A:186:ILE:HD13	1:A:216:GLU:HA	1.95	0.49
1:A:144:THR:HG22	1:A:146:LYS:HG3	1.94	0.49
1:A:12:LEU:HD22	1:A:325:TRP:HZ3	1.78	0.49
1:A:352:GLN:O	1:A:356:MET:HB2	2.12	0.49
1:B:164:LEU:C	1:B:164:LEU:HD23	2.34	0.49
1:A:218:ILE:CG2	1:A:222:LYS:HE3	2.43	0.48
1:A:325:TRP:O	1:A:329:CYS:HB2	2.13	0.48
1:B:44:ASN:ND2	1:B:46:ASN:H	2.11	0.48
1:A:448:LEU:HB3	1:A:458:LEU:HG	1.96	0.48
1:B:405:PHE:HB3	1:B:428:PHE:CE1	2.49	0.48
1:B:514:VAL:CG2	1:B:518:LYS:HE3	2.44	0.48
1:B:458:LEU:C	1:B:458:LEU:HD23	2.34	0.48
1:B:171:LYS:HD3	1:B:286:HIS:HE1	1.78	0.48
1:A:42:THR:HG22	1:A:51:LEU:HD13	1.95	0.48
1:B:325:TRP:O	1:B:329:CYS:HB2	2.14	0.48
1:A:388:HIS:HE2	1:B:216:GLU:CD	2.18	0.47
1:B:19:HIS:O	1:B:22:GLU:HB3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:246:SER:OG	1:A:247:THR:N	2.47	0.47
1:A:218:ILE:HG22	1:A:222:LYS:HE3	1.96	0.47
1:A:120:GLU:HB2	2:A:699:HOH:O	2.14	0.47
1:A:445:ARG:CG	1:A:449:GLN:HE21	2.23	0.47
1:B:61:GLU:HG3	2:B:731:HOH:O	2.15	0.47
1:B:530:GLY:O	1:B:552:ARG:NH2	2.48	0.46
1:A:12:LEU:HD22	1:A:325:TRP:CZ3	2.50	0.46
1:A:312:GLU:CD	1:A:312:GLU:H	2.19	0.46
1:A:144:THR:O	1:A:144:THR:HG23	2.15	0.46
1:A:420:HIS:HD2	1:B:186:ILE:O	1.99	0.46
1:A:90:ASN:HD22	1:A:90:ASN:C	2.19	0.46
1:A:518:LYS:HZ2	1:A:518:LYS:HB2	1.80	0.46
1:B:25:LEU:HB3	1:B:436:MET:HG2	1.98	0.45
1:A:248:ASN:O	1:A:252:VAL:HG23	2.15	0.45
1:B:209:SER:O	1:B:246:SER:HB2	2.17	0.45
1:B:7:PRO:HG2	1:B:8:GLN:NE2	2.31	0.45
1:B:152:ILE:N	1:B:152:ILE:HD12	2.32	0.45
1:A:303:ASP:OD1	1:A:495:HIS:CE1	2.69	0.45
1:A:8:GLN:HE21	1:A:73:SER:CB	2.29	0.45
1:A:345:HIS:CA	1:A:382:PRO:HG3	2.33	0.45
1:A:216:GLU:OE2	1:B:388:HIS:NE2	2.49	0.44
1:A:515:GLU:HG3	2:A:683:HOH:O	2.17	0.44
1:B:99:HIS:HD2	2:B:576:HOH:O	2.00	0.44
1:B:6:ASN:ND2	1:B:8:GLN:N	2.65	0.44
1:A:534:VAL:HG23	1:A:549:LYS:HE3	2.00	0.44
1:A:405:PHE:HB3	1:A:428:PHE:CE1	2.53	0.44
1:A:422:LYS:HE3	1:B:525:GLU:O	2.18	0.44
1:B:522:LYS:HE2	2:B:872:HOH:O	2.18	0.44
1:A:516:LEU:HD13	1:B:434:ALA:HB1	2.00	0.43
1:A:289:PHE:O	1:A:293:GLU:HG3	2.18	0.43
1:B:8:GLN:HE21	1:B:73:SER:CB	2.31	0.43
1:A:116:ASP:OD2	1:A:119:PRO:HD3	2.18	0.43
1:A:445:ARG:O	1:A:449:GLN:HG3	2.19	0.43
1:A:387:GLN:HA	1:A:391:TYR:CG	2.54	0.43
1:A:111:VAL:HG13	1:A:115:LYS:N	2.33	0.43
1:B:312:GLU:N	1:B:312:GLU:CD	2.67	0.43
1:B:210:LYS:HG2	1:B:265:PHE:CZ	2.53	0.43
1:B:387:GLN:HA	1:B:391:TYR:CE1	2.53	0.43
1:A:74:ARG:HH21	1:A:505:ASP:HB2	1.82	0.43
1:B:246:SER:OG	1:B:247:THR:N	2.52	0.43
1:B:99:HIS:H	1:B:99:HIS:CD2	2.36	0.43
1:B:234:ASP:OD1	1:B:234:ASP:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:HIS:HE1	2:B:925:HOH:O	2.00	0.43
1:B:343:TYR:OH	1:B:413:HIS:CE1	2.69	0.43
1:A:518:LYS:NZ	1:A:518:LYS:CB	2.82	0.43
1:B:407:ILE:O	1:B:407:ILE:HG23	2.18	0.43
1:B:156:ILE:CG1	2:B:816:HOH:O	2.51	0.43
1:A:99:HIS:HE1	2:A:586:HOH:O	2.01	0.42
1:A:25:LEU:HB3	1:A:436:MET:HG2	2.01	0.42
1:A:407:ILE:HD13	1:A:425:LEU:HD23	2.01	0.42
1:A:251:LYS:HD3	1:A:251:LYS:HA	1.84	0.42
1:A:490:ILE:O	1:A:494:GLU:HG3	2.20	0.42
1:B:305:HIS:HE1	1:B:315:ALA:N	2.06	0.42
1:B:210:LYS:CG	1:B:265:PHE:CE1	3.02	0.42
1:B:191:ILE:HG13	1:B:195:LEU:HD22	2.02	0.42
1:A:245:LEU:HD13	1:A:279:ILE:HA	2.01	0.42
1:A:530:GLY:O	1:A:552:ARG:NH2	2.52	0.42
1:B:218:ILE:O	1:B:222:LYS:HG3	2.20	0.42
1:A:99:HIS:HD2	2:A:610:HOH:O	2.02	0.42
1:A:274:SER:O	1:A:279:ILE:HB	2.20	0.42
1:A:144:THR:CG2	1:A:146:LYS:HG3	2.49	0.41
1:A:195:LEU:HD13	1:A:227:TRP:CG	2.55	0.41
1:B:80:ARG:HD2	1:B:307:ARG:HA	2.01	0.41
1:A:6:ASN:HA	1:A:7:PRO:HD3	1.88	0.41
2:A:832:HOH:O	1:B:514:VAL:HG23	2.20	0.41
1:A:123:LYS:O	1:A:123:LYS:HD3	2.21	0.41
1:A:352:GLN:HG2	1:A:378:VAL:O	2.21	0.41
1:A:99:HIS:CD2	1:A:99:HIS:H	2.39	0.41
1:B:248:ASN:O	1:B:252:VAL:HG23	2.21	0.41
1:A:72:LYS:HG2	1:A:311:LEU:HD12	2.03	0.41
1:B:490:ILE:O	1:B:494:GLU:HG3	2.21	0.41
1:B:283:ILE:O	1:B:287:VAL:HG22	2.21	0.41
1:B:550:GLN:NE2	1:B:551:GLN:HE21	2.05	0.40
1:A:161:LEU:CD2	1:A:350:TYR:HA	2.52	0.40
1:B:186:ILE:HD13	1:B:216:GLU:HA	2.03	0.40
1:A:445:ARG:HG2	1:A:449:GLN:NE2	2.24	0.40
1:B:171:LYS:NZ	1:B:286:HIS:CE1	2.89	0.40
1:A:443:GLU:O	1:A:447:GLU:HG3	2.21	0.40
1:A:171:LYS:NZ	1:A:286:HIS:CE1	2.90	0.40
1:A:369:ARG:NH1	1:A:369:ARG:HG2	2.34	0.40
1:A:41:LEU:HD12	1:A:41:LEU:C	2.42	0.40
1:B:99:HIS:HE1	2:B:612:HOH:O	2.04	0.40
1:B:253:LYS:NZ	1:B:253:LYS:CB	2.85	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	554/558 (99%)	535 (97%)	18 (3%)	1 (0%)	56	38
1	B	554/558 (99%)	533 (96%)	19 (3%)	2 (0%)	43	25
All	All	1108/1116 (99%)	1068 (96%)	37 (3%)	3 (0%)	50	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	384	THR
1	A	384	THR
1	B	20	GLY

### 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	477/479 (100%)	459 (96%)	18 (4%)	44	24
1	B	477/479 (100%)	468 (98%)	9 (2%)	69	56
All	All	954/958 (100%)	927 (97%)	27 (3%)	56	38

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

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	ARG
1	A	22	GLU
1	A	90	ASN
1	A	103	ARG
1	A	144	THR

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Mol	Chain	Res	Type
1	A	175	SER
1	A	212	PHE
1	A	229	LEU
1	A	289	PHE
1	A	442	GLU
1	A	448	LEU
1	A	460	LYS
1	A	511	GLN
1	A	515	GLU
1	A	516	LEU
1	A	518	LYS
1	A	552	ARG
1	B	44	ASN
1	B	58	LEU
1	B	90	ASN
1	B	103	ARG
1	B	133	GLN
1	B	195	LEU
1	B	289	PHE
1	B	459	MET
1	B	511	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	13	GLN
1	A	14	GLN
1	A	49	HIS
1	A	90	ASN
1	A	99	HIS
1	A	153	ASN
1	A	215	GLN
1	A	260	GLN
1	A	286	HIS
1	A	294	GLN
1	A	304	GLN
1	A	352	GLN
1	A	353	GLN
1	A	387	GLN
1	A	410	GLN
1	A	420	HIS

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Mol	Chain	Res	Type
1	A	449	GLN
1	A	495	HIS
1	A	511	GLN
1	A	542	ASN
1	A	550	GLN
1	B	6	ASN
1	B	8	GLN
1	B	10	GLN
1	B	16	HIS
1	B	44	ASN
1	B	49	HIS
1	B	65	HIS
1	B	90	ASN
1	B	99	HIS
1	B	153	ASN
1	B	215	GLN
1	B	286	HIS
1	B	304	GLN
1	B	305	HIS
1	B	353	GLN
1	B	359	ASN
1	B	387	GLN
1	B	395	HIS
1	B	413	HIS
1	B	420	HIS
1	B	449	GLN
1	B	495	HIS
1	B	511	GLN
1	B	542	ASN
1	B	550	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	556/558 (99%)	-0.02	14 (2%) 54 47	14, 25, 43, 52	0
1	B	556/558 (99%)	-0.13	8 (1%) 72 68	14, 23, 39, 52	0
All	All	1112/1116 (99%)	-0.08	22 (1%) 62 56	14, 24, 41, 52	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ARG	3.8
1	A	2	ALA	3.7
1	A	22	GLU	3.2
1	A	17	ARG	3.1
1	A	384	THR	3.1
1	A	114	GLY	2.7
1	B	553	GLU	2.6
1	B	114	GLY	2.6
1	A	553	GLU	2.6
1	B	22	GLU	2.5
1	A	115	LYS	2.4
1	A	449	GLN	2.4
1	B	232	ALA	2.3
1	B	384	THR	2.3
1	B	556	ILE	2.3
1	A	14	GLN	2.2
1	A	383	GLY	2.2
1	A	230	LEU	2.1
1	B	260	GLN	2.1
1	A	555	LYS	2.1
1	A	556	ILE	2.0
1	B	17	ARG	2.0



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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.