



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:10 PM GMT

PDB ID : 1PMI  
Title : Candida Albicans Phosphomannose Isomerase  
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Deposited on : 1996-04-03  
Resolution : 1.70 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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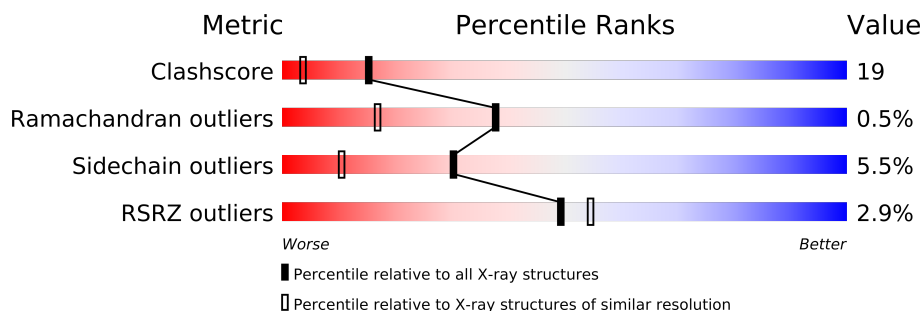
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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))
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (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. 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	440	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3754 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 PHOSPHOMANNOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3431	2181	568	670	12			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

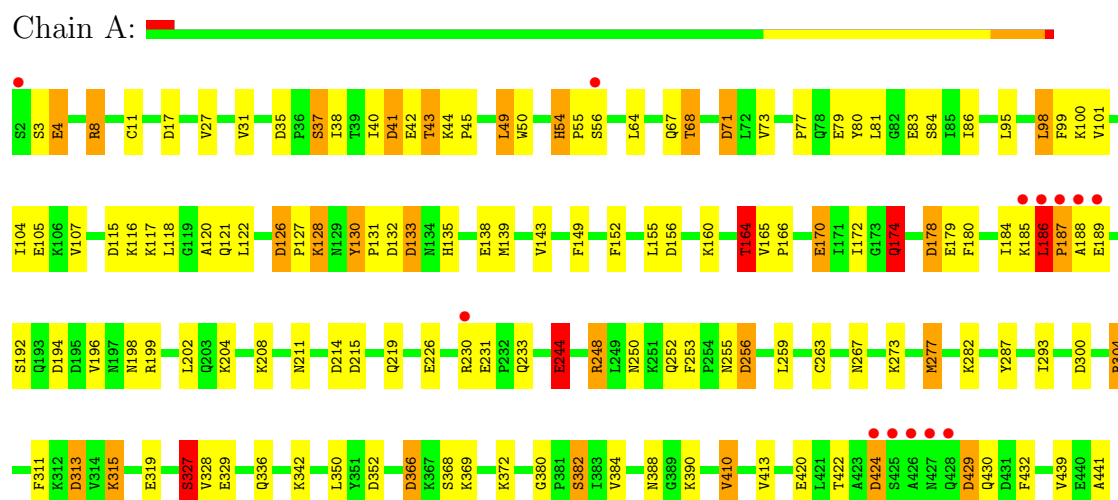
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	322	Total	O	0	0
			322	322		

### 3 Residue-property plots

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: PHOSPHOMANNOSE ISOMERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.83Å 52.92Å 85.73Å 90.00° 127.54° 90.00°	Depositor
Resolution (Å)	7.00 – 1.70 19.79 – 1.66	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.70) 86.4 (19.79-1.66)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.25 (at 1.66Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.184 , (Not available) 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 66.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 45325 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% 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

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

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	1.28	11/3499 (0.3%)	1.65	50/4734 (1.1%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	ARG	CG-CD	-9.62	1.27	1.51
1	A	199	ARG	CD-NE	-9.50	1.30	1.46
1	A	441	ALA	C-O	7.32	1.37	1.23
1	A	164	THR	CA-CB	6.72	1.70	1.53
1	A	133	ASP	CA-CB	6.41	1.68	1.53
1	A	277	MET	CG-SD	6.25	1.97	1.81
1	A	170	GLU	CD-OE2	-5.84	1.19	1.25
1	A	382	SER	CB-OG	-5.47	1.35	1.42
1	A	139	MET	CG-SD	5.32	1.95	1.81
1	A	244	GLU	CD-OE1	5.22	1.31	1.25
1	A	319	GLU	CB-CG	5.09	1.61	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	CD-NE-CZ	35.97	173.95	123.60
1	A	199	ARG	CG-CD-NE	16.15	145.72	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	CB-CG-CD	12.26	143.47	111.60
1	A	17	ASP	CB-CG-OD1	9.47	126.83	118.30
1	A	126	ASP	CB-CG-OD1	8.91	126.32	118.30
1	A	429	ASP	CB-CG-OD1	-8.52	110.63	118.30
1	A	199	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	A	99	PHE	CB-CG-CD2	-8.19	115.06	120.80
1	A	152	PHE	CB-CG-CD1	-7.73	115.39	120.80
1	A	130	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	A	132	ASP	C-N-CA	7.49	140.44	121.70
1	A	8	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	138	GLU	OE1-CD-OE2	6.86	131.54	123.30
1	A	115	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	441	ALA	CA-C-O	-6.84	105.74	120.10
1	A	4	GLU	CB-CG-CD	6.78	132.51	114.20
1	A	170	GLU	CG-CD-OE1	-6.75	104.80	118.30
1	A	174	GLN	CA-CB-CG	6.67	128.07	113.40
1	A	304	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	429	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	327	SER	CB-CA-C	-6.23	98.27	110.10
1	A	71	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	A	248	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	164	THR	CA-CB-OG1	-5.96	96.49	109.00
1	A	8	ARG	CD-NE-CZ	5.81	131.74	123.60
1	A	256	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	282	LYS	CB-CG-CD	5.66	126.32	111.60
1	A	170	GLU	CA-CB-CG	5.64	125.82	113.40
1	A	156	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	A	313	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	133	ASP	N-CA-CB	-5.55	100.61	110.60
1	A	105	GLU	CG-CD-OE2	5.42	129.14	118.30
1	A	54	HIS	CA-CB-CG	-5.40	104.42	113.60
1	A	214	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	180	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	A	366	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	A	248	ARG	CD-NE-CZ	-5.31	116.17	123.60
1	A	164	THR	N-CA-CB	-5.30	100.23	110.30
1	A	186	LEU	CA-CB-CG	-5.30	103.12	115.30
1	A	149	PHE	CB-CG-CD1	-5.27	117.11	120.80
1	A	8	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	432	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	A	99	PHE	CB-CG-CD1	5.19	124.43	120.80
1	A	17	ASP	CB-CG-OD2	-5.18	113.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	GLU	CA-CB-CG	5.17	124.78	113.40
1	A	424	ASP	CA-CB-CG	-5.15	102.07	113.40
1	A	41	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	420	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	A	133	ASP	CA-CB-CG	-5.05	102.28	113.40
1	A	4	GLU	CG-CD-OE1	5.00	128.31	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ARG	Sidechain
1	A	304	ARG	Sidechain
1	A	8	ARG	Sidechain

## 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	3431	0	3418	129	0
2	A	1	0	0	0	0
3	A	322	0	0	33	1
All	All	3754	0	3418	129	1

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 19.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:352:ASP:HB2	3:A:844:HOH:O	1.44	1.16
1:A:352:ASP:CB	3:A:844:HOH:O	1.94	1.13
1:A:128:LYS:CD	1:A:128:LYS:H	1.53	1.13
1:A:127:PRO:HG2	1:A:128:LYS:HE2	1.40	1.03
1:A:68:THR:HG22	1:A:71:ASP:H	1.21	1.03
1:A:64:LEU:O	1:A:67:GLN:HG3	1.60	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:LYS:HD2	1:A:128:LYS:N	1.58	1.00
1:A:35:ASP:OD1	1:A:37:SER:HB3	1.63	0.96
1:A:3:SER:HB3	3:A:713:HOH:O	1.66	0.95
1:A:73:VAL:HG13	1:A:81:LEU:CD1	1.98	0.93
1:A:128:LYS:HD2	1:A:128:LYS:H	0.79	0.93
1:A:352:ASP:CA	3:A:844:HOH:O	2.16	0.91
1:A:233:GLN:HG2	3:A:919:HOH:O	1.76	0.84
1:A:127:PRO:HD2	1:A:128:LYS:HE3	1.60	0.81
1:A:160:LYS:O	1:A:164:THR:HB	1.80	0.81
1:A:73:VAL:HG13	1:A:81:LEU:HD11	1.62	0.81
1:A:126:ASP:HA	1:A:128:LYS:HE3	1.62	0.80
1:A:164:THR:HG21	3:A:823:HOH:O	1.81	0.79
1:A:127:PRO:CD	1:A:128:LYS:HE3	2.12	0.79
1:A:68:THR:HG21	3:A:659:HOH:O	1.82	0.78
1:A:127:PRO:CG	1:A:128:LYS:HE2	2.13	0.78
1:A:126:ASP:OD1	1:A:128:LYS:HD3	1.86	0.76
1:A:73:VAL:CG1	1:A:81:LEU:HD11	2.16	0.76
1:A:131:PRO:HG3	1:A:300:ASP:CB	2.15	0.75
1:A:174:GLN:O	1:A:178:ASP:HB2	1.87	0.75
1:A:11:CYS:HB2	1:A:49:LEU:HD21	1.68	0.74
1:A:131:PRO:HG3	1:A:300:ASP:HB2	1.69	0.73
1:A:83:GLU:HG3	1:A:84:SER:H	1.53	0.72
1:A:98:LEU:HD13	1:A:100:LYS:HE3	1.68	0.72
1:A:230:ARG:NH1	1:A:231:GLU:OE2	2.23	0.72
1:A:107:VAL:H	1:A:252:GLN:HE22	1.35	0.72
1:A:186:LEU:O	1:A:188:ALA:N	2.24	0.71
1:A:174:GLN:HB2	3:A:647:HOH:O	1.91	0.69
1:A:230:ARG:HD3	3:A:867:HOH:O	1.91	0.69
1:A:79:GLU:HG2	3:A:882:HOH:O	1.93	0.69
1:A:116:LYS:HG2	3:A:592:HOH:O	1.92	0.68
1:A:267:ASN:HB3	1:A:328:VAL:HG22	1.75	0.67
1:A:204:LYS:HD3	3:A:869:HOH:O	1.94	0.67
1:A:42:GLU:HA	1:A:42:GLU:OE1	1.94	0.67
1:A:336:GLN:OE1	3:A:938:HOH:O	2.12	0.67
1:A:244:GLU:HB3	3:A:821:HOH:O	1.94	0.67
1:A:68:THR:HG22	1:A:71:ASP:N	2.02	0.66
1:A:118:LEU:O	1:A:122:LEU:HD13	1.96	0.66
1:A:179:GLU:OE2	1:A:204:LYS:NZ	2.28	0.66
1:A:4:GLU:HG2	1:A:80:TYR:OH	1.96	0.65
1:A:127:PRO:CD	1:A:128:LYS:CE	2.74	0.64
1:A:233:GLN:OE1	1:A:233:GLN:HA	1.97	0.63
1:A:327:SER:HB2	1:A:329:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:342:LYS:HG3	3:A:716:HOH:O	1.99	0.63
1:A:54:HIS:ND1	1:A:56:SER:OG	2.28	0.62
1:A:3:SER:CB	3:A:713:HOH:O	2.36	0.61
1:A:390:LYS:HG3	1:A:424:ASP:HB2	1.83	0.61
1:A:185:LYS:HB2	1:A:194:ASP:HB3	1.83	0.60
1:A:311:PHE:CE2	1:A:313:ASP:HB2	2.39	0.58
1:A:131:PRO:HG3	1:A:300:ASP:HB3	1.85	0.58
1:A:41:ASP:OD1	1:A:43:THR:HB	2.04	0.58
1:A:116:LYS:HG3	3:A:598:HOH:O	2.05	0.57
1:A:73:VAL:HG13	1:A:81:LEU:HD13	1.85	0.57
1:A:143:VAL:O	1:A:273:LYS:HE3	2.05	0.56
1:A:44:LYS:HG2	1:A:45:PRO:HD2	1.88	0.56
1:A:131:PRO:CG	1:A:300:ASP:HB2	2.36	0.56
1:A:424:ASP:HA	3:A:843:HOH:O	2.07	0.55
1:A:107:VAL:H	1:A:252:GLN:NE2	2.04	0.54
1:A:186:LEU:HB3	1:A:187:PRO:HD3	1.89	0.54
1:A:128:LYS:CD	1:A:128:LYS:N	2.35	0.54
1:A:127:PRO:HG2	1:A:128:LYS:CE	2.25	0.54
1:A:104:ILE:HD13	1:A:287:TYR:HB3	1.89	0.54
1:A:184:ILE:HA	1:A:198:ASN:OD1	2.08	0.53
1:A:77:PRO:HB2	1:A:86:ILE:HD11	1.91	0.52
1:A:350:LEU:HG	3:A:844:HOH:O	2.08	0.52
1:A:233:GLN:HG2	3:A:918:HOH:O	2.09	0.52
1:A:127:PRO:CG	1:A:128:LYS:CE	2.86	0.51
1:A:315:LYS:HE3	1:A:315:LYS:O	2.11	0.51
1:A:128:LYS:NZ	3:A:725:HOH:O	2.42	0.51
1:A:127:PRO:N	1:A:128:LYS:HE3	2.26	0.51
1:A:107:VAL:HG12	1:A:252:GLN:NE2	2.26	0.51
1:A:372:LYS:HG2	1:A:422:THR:HG22	1.93	0.51
1:A:54:HIS:CE1	1:A:56:SER:OG	2.65	0.50
1:A:83:GLU:HG3	1:A:84:SER:N	2.22	0.50
1:A:116:LYS:CG	3:A:592:HOH:O	2.55	0.49
1:A:439:VAL:HG23	3:A:676:HOH:O	2.12	0.49
1:A:366:ASP:HB3	1:A:369:LYS:HB3	1.94	0.49
1:A:244:GLU:CD	3:A:790:HOH:O	2.51	0.49
1:A:215:ASP:O	1:A:219:GLN:HG3	2.14	0.48
1:A:250:ASN:ND2	1:A:255:ASN:H	2.12	0.47
1:A:130:TYR:HA	1:A:131:PRO:HD2	1.74	0.47
1:A:120:ALA:HA	1:A:133:ASP:OD1	2.14	0.47
1:A:127:PRO:HD2	1:A:128:LYS:CE	2.36	0.47
1:A:54:HIS:CE1	1:A:56:SER:HG	2.29	0.47
1:A:369:LYS:HG2	3:A:880:HOH:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:54:HIS:CE1	1:A:55:PRO:HD2	2.50	0.46
1:A:164:THR:CG2	3:A:823:HOH:O	2.50	0.46
1:A:388:ASN:HD22	1:A:430:GLN:HE22	1.63	0.46
1:A:430:GLN:OE1	3:A:931:HOH:O	2.20	0.46
1:A:44:LYS:CG	1:A:45:PRO:HD2	2.46	0.46
1:A:380:GLY:HA3	1:A:439:VAL:O	2.15	0.46
1:A:172:ILE:O	1:A:208:LYS:HD3	2.17	0.45
1:A:127:PRO:N	1:A:128:LYS:CE	2.79	0.45
1:A:4:GLU:CG	1:A:80:TYR:OH	2.63	0.45
1:A:186:LEU:HD22	1:A:186:LEU:HA	1.25	0.44
1:A:116:LYS:CD	3:A:592:HOH:O	2.64	0.44
1:A:27:VAL:O	1:A:31:VAL:HG23	2.17	0.44
1:A:211:ASN:HB3	3:A:936:HOH:O	2.16	0.44
1:A:352:ASP:HA	3:A:844:HOH:O	2.01	0.44
1:A:11:CYS:CB	1:A:49:LEU:HD21	2.41	0.44
1:A:35:ASP:HB3	1:A:38:ILE:HD12	2.00	0.44
1:A:259:LEU:O	1:A:263:CYS:HB2	2.17	0.44
1:A:11:CYS:HB3	1:A:50:TRP:O	2.18	0.43
1:A:230:ARG:HH11	1:A:230:ARG:HG2	1.82	0.43
1:A:250:ASN:HD22	1:A:259:LEU:HD11	1.83	0.43
1:A:107:VAL:HG12	1:A:252:GLN:HE21	1.82	0.43
1:A:164:THR:HG22	1:A:165:VAL:HG23	2.00	0.43
1:A:116:LYS:HD3	3:A:592:HOH:O	2.19	0.43
1:A:117:LYS:O	1:A:121:GLN:HG3	2.18	0.43
1:A:369:LYS:CE	3:A:576:HOH:O	2.67	0.43
1:A:253:PHE:HB3	1:A:256:ASP:HB2	2.01	0.43
1:A:166:PRO:O	1:A:170:GLU:HB2	2.19	0.42
1:A:342:LYS:HD3	3:A:651:HOH:O	2.19	0.42
1:A:384:VAL:O	1:A:410:VAL:HA	2.20	0.42
1:A:101:VAL:HG22	1:A:293:ILE:HD13	2.00	0.42
1:A:336:GLN:HE22	1:A:352:ASP:HB3	1.85	0.42
1:A:73:VAL:HG11	1:A:81:LEU:HD11	1.96	0.42
1:A:192:SER:O	1:A:196:VAL:HG23	2.21	0.41
1:A:382:SER:HB2	1:A:413:VAL:HB	2.01	0.41
1:A:118:LEU:HD11	1:A:122:LEU:HD11	2.02	0.41
1:A:155:LEU:HD21	1:A:198:ASN:HB3	2.02	0.41
1:A:366:ASP:OD2	1:A:368:SER:HB2	2.21	0.40
1:A:186:LEU:HD13	1:A:186:LEU:C	2.41	0.40
1:A:390:LYS:HG3	1:A:424:ASP:CB	2.50	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	Distance(Å)	Clash(Å)
3:A:827:HOH:O	3:A:835:HOH:O[4_647]	2.04	0.16

## 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	438/440 (100%)	426 (97%)	10 (2%)	2 (0%)	38 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	PRO
1	A	186	LEU

### 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	382/382 (100%)	361 (94%)	21 (6%)	30 10

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	40	ILE
1	A	43	THR
1	A	49	LEU
1	A	68	THR
1	A	95	LEU
1	A	98	LEU
1	A	128	LYS

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	135	HIS
1	A	164	THR
1	A	174	GLN
1	A	178	ASP
1	A	186	LEU
1	A	202	LEU
1	A	226	GLU
1	A	244	GLU
1	A	277	MET
1	A	315	LYS
1	A	327	SER
1	A	410	VAL
1	A	429	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	129	ASN
1	A	157	GLN
1	A	193	GLN
1	A	247	GLN
1	A	250	ASN
1	A	252	GLN
1	A	336	GLN
1	A	430	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 ⓘ

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.

## 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	440/440 (100%)	-0.06	13 (2%) 48 53	8, 19, 41, 65	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	ASN	6.2
1	A	186	LEU	5.6
1	A	188	ALA	3.5
1	A	428	GLN	2.9
1	A	230	ARG	2.7
1	A	189	GLU	2.6
1	A	185	LYS	2.2
1	A	2	SER	2.2
1	A	56	SER	2.2
1	A	426	ALA	2.2
1	A	425	SER	2.1
1	A	424	ASP	2.1
1	A	187	PRO	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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	445	1/1	0.03	-1.64	12,12,12,12	0

## 6.5 Other polymers

There are no such residues in this entry.