



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:02 PM UTC

PDB ID : 1PMI / pdb_00001pmi
Title : Candida Albicans Phosphomannose Isomerase
Authors : Cleasby, A.; Skarzynski, T.; Wonacott, A.; Davies, G.J.; Hubbard, R.E.; Proudfoot, A.E.I.; Wells, T.N.C.; Payton, M.A.; Bernard, A.R.
Deposited on : 1996-04-03
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

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

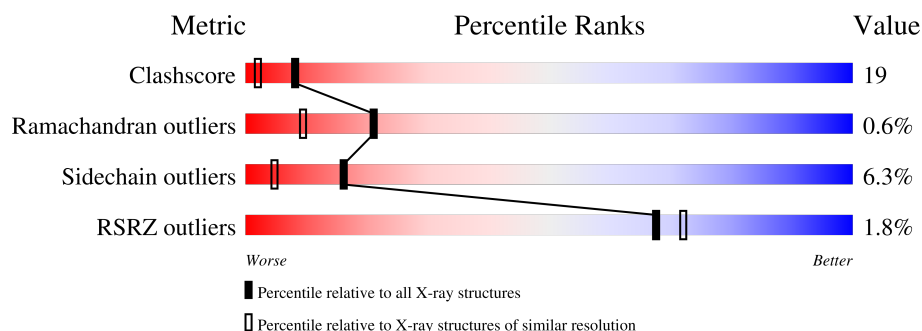
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	440	2% 63% 27% 9% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3754 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 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 (CCD ID: ZN) (formula: Zn).

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

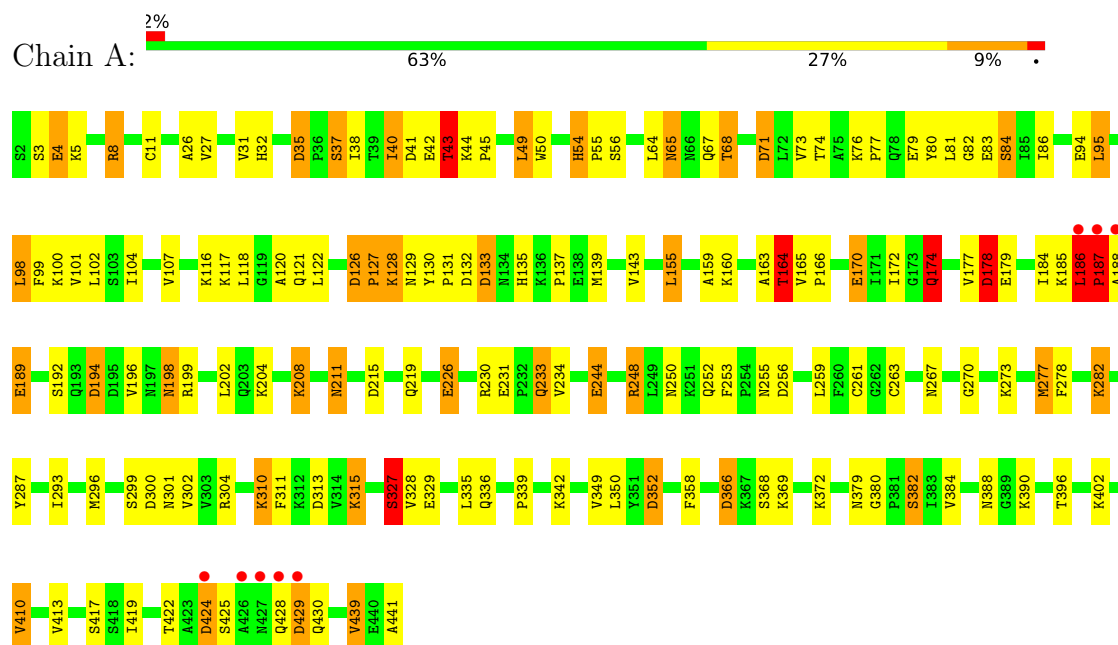
- Molecule 3 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PHOSPHOMANNOSE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.83Å 52.92Å 85.73Å 90.00° 127.54° 90.00°	Depositor
Resolution (Å)	7.00 – 1.70 7.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.70) 86.0 (7.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 1.66Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.184 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 84.9	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	0.96	EDS
Total number of atoms	3754	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	1.59	25/3499 (0.7%)	1.99	92/4734 (1.9%)

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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	ARG	CD-NE	-11.40	1.30	1.46
1	A	164	THR	CA-CB	10.42	1.70	1.53
1	A	133	ASP	CA-CB	8.29	1.68	1.53
1	A	199	ARG	CG-CD	-8.18	1.27	1.52
1	A	270	GLY	CA-C	7.72	1.58	1.52
1	A	187	PRO	CA-CB	-7.20	1.43	1.53
1	A	43	THR	CA-CB	6.95	1.65	1.53
1	A	133	ASP	N-CA	-6.87	1.36	1.46
1	A	441	ALA	C-O	6.86	1.37	1.23
1	A	277	MET	CG-SD	6.66	1.97	1.80
1	A	419	ILE	CA-CB	6.55	1.63	1.54
1	A	186	LEU	C-O	6.35	1.32	1.24
1	A	417	SER	C-O	6.24	1.31	1.24
1	A	159	ALA	C-O	6.19	1.31	1.24
1	A	139	MET	CG-SD	5.69	1.95	1.80
1	A	189	GLU	N-CA	5.67	1.52	1.45
1	A	299	SER	C-N	-5.54	1.25	1.33
1	A	352	ASP	CA-CB	5.39	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	VAL	CA-CB	5.38	1.61	1.54
1	A	339	PRO	C-O	5.37	1.30	1.24
1	A	102	LEU	N-CA	5.30	1.52	1.46
1	A	159	ALA	N-CA	5.25	1.52	1.46
1	A	137	PRO	C-O	5.24	1.29	1.23
1	A	187	PRO	N-CA	5.15	1.53	1.47
1	A	26	ALA	N-CA	5.06	1.52	1.46

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	CD-NE-CZ	35.39	173.95	124.40
1	A	199	ARG	CG-CD-NE	15.33	145.72	112.00
1	A	199	ARG	CB-CG-CD	13.99	143.47	111.30
1	A	4	GLU	CB-CG-CD	11.71	132.51	112.60
1	A	132	ASP	CA-C-N	10.85	140.44	122.54
1	A	132	ASP	C-N-CA	10.85	140.44	122.54
1	A	424	ASP	CA-CB-CG	-10.53	102.07	112.60
1	A	133	ASP	CA-CB-CG	-10.32	102.28	112.60
1	A	54	HIS	CA-CB-CG	-9.38	104.42	113.80
1	A	441	ALA	CA-C-O	-8.86	105.74	120.80
1	A	164	THR	CA-CB-OG1	-8.74	96.49	109.60
1	A	352	ASP	O-C-N	8.61	129.95	120.83
1	A	32	HIS	CA-CB-CG	-8.42	105.38	113.80
1	A	226	GLU	CB-CG-CD	8.35	126.80	112.60
1	A	71	ASP	CA-CB-CG	-8.28	104.32	112.60
1	A	178	ASP	CA-CB-CG	-7.78	104.82	112.60
1	A	177	VAL	CA-C-O	7.71	129.34	121.17
1	A	194	ASP	CA-C-O	-7.69	112.26	120.42
1	A	211	ASN	CA-CB-CG	-7.61	105.00	112.60
1	A	352	ASP	CA-C-O	-7.56	113.41	119.99
1	A	194	ASP	O-C-N	7.46	130.66	122.15
1	A	429	ASP	CA-CB-CG	-7.44	105.16	112.60
1	A	402	LYS	CA-C-O	7.16	128.89	120.58
1	A	164	THR	N-CA-C	7.14	122.08	113.23
1	A	99	PHE	CA-CB-CG	7.07	120.86	113.80
1	A	174	GLN	CA-CB-CG	6.98	128.07	114.10
1	A	234	VAL	O-C-N	6.82	128.48	121.87
1	A	299	SER	CA-C-N	6.73	132.78	122.29
1	A	299	SER	C-N-CA	6.73	132.78	122.29
1	A	299	SER	CA-C-O	-6.68	114.11	121.33
1	A	133	ASP	N-CA-CB	-6.67	100.61	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ASN	CA-CB-CG	-6.66	105.94	112.60
1	A	396	THR	O-C-N	6.66	131.06	123.06
1	A	71	ASP	CA-C-O	-6.64	113.85	120.82
1	A	164	THR	N-CA-CB	-6.55	100.23	110.44
1	A	282	LYS	CB-CG-CD	6.53	126.32	111.30
1	A	187	PRO	CB-CA-C	6.41	122.14	111.56
1	A	127	PRO	CA-C-N	6.34	129.30	120.29
1	A	127	PRO	C-N-CA	6.34	129.30	120.29
1	A	379	ASN	OD1-CG-ND2	6.33	128.93	122.60
1	A	74	THR	O-C-N	6.26	128.52	122.07
1	A	352	ASP	CB-CA-C	-6.24	103.96	110.33
1	A	174	GLN	CB-CG-CD	6.23	123.19	112.60
1	A	198	ASN	CA-CB-CG	6.16	118.75	112.60
1	A	327	SER	CB-CA-C	-6.11	98.27	110.42
1	A	282	LYS	CG-CD-CE	6.05	125.22	111.30
1	A	302	VAL	O-C-N	5.96	129.66	123.05
1	A	170	GLU	CG-CD-OE1	-5.91	104.80	118.40
1	A	5	LYS	CA-C-N	5.90	130.99	122.44
1	A	5	LYS	C-N-CA	5.90	130.99	122.44
1	A	248	ARG	CD-NE-CZ	-5.88	116.17	124.40
1	A	40	ILE	CB-CA-C	5.86	118.77	111.15
1	A	301	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	A	170	GLU	CA-CB-CG	5.86	125.82	114.10
1	A	199	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	A	379	ASN	CA-CB-CG	-5.76	106.84	112.60
1	A	299	SER	N-CA-C	-5.74	100.34	109.07
1	A	187	PRO	N-CA-C	-5.70	100.74	112.47
1	A	164	THR	OG1-CB-CG2	5.68	120.67	109.30
1	A	428	GLN	CB-CG-CD	-5.65	103.00	112.60
1	A	163	ALA	CA-C-N	5.63	131.57	121.66
1	A	163	ALA	C-N-CA	5.63	131.57	121.66
1	A	366	ASP	CA-CB-CG	-5.50	107.09	112.60
1	A	382	SER	O-C-N	5.46	129.60	123.27
1	A	95	LEU	O-C-N	5.41	127.48	121.53
1	A	208	LYS	CA-CB-CG	-5.41	103.28	114.10
1	A	84	SER	O-C-N	5.40	128.54	122.22
1	A	425	SER	CB-CA-C	5.38	119.24	110.96
1	A	233	GLN	CB-CG-CD	-5.36	103.49	112.60
1	A	189	GLU	CA-CB-CG	5.34	124.78	114.10
1	A	177	VAL	CA-C-N	5.33	127.74	120.54
1	A	177	VAL	C-N-CA	5.33	127.74	120.54
1	A	126	ASP	CA-C-N	5.33	125.14	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	C-N-CA	5.33	125.14	119.28
1	A	35	ASP	O-C-N	5.30	124.94	121.23
1	A	43	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	8	ARG	CD-NE-CZ	5.24	131.74	124.40
1	A	194	ASP	N-CA-CB	5.17	117.82	110.16
1	A	40	ILE	CB-CG1-CD1	5.15	124.62	113.80
1	A	133	ASP	N-CA-C	5.13	119.63	113.17
1	A	94	GLU	N-CA-C	5.12	116.58	108.96
1	A	278	PHE	CA-C-O	-5.11	114.86	120.43
1	A	439	VAL	O-C-N	5.09	128.99	123.09
1	A	335	LEU	CA-C-O	-5.08	114.96	120.81
1	A	76	LYS	CA-C-N	5.08	124.69	119.05
1	A	76	LYS	C-N-CA	5.08	124.69	119.05
1	A	358	PHE	CA-C-N	5.07	130.82	121.85
1	A	358	PHE	C-N-CA	5.07	130.82	121.85
1	A	82	GLY	N-CA-C	-5.07	106.35	112.48
1	A	261	CYS	CA-C-O	-5.07	113.15	119.38
1	A	310	LYS	CA-CB-CG	5.02	124.15	114.10
1	A	65	ASN	N-CA-CB	-5.00	104.86	112.47

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 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	3431	0	3420	133	0
2	A	1	0	0	0	0
3	A	322	0	0	34	1
All	All	3754	0	3420	133	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 19.

All (133) 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:352:ASP:HB2	3:A:844:HOH:O	1.44	1.16
1:A:128:LYS:H	1:A:128:LYS:CD	1.53	1.13
1:A:352:ASP:CB	3:A:844:HOH:O	1.94	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
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:H	1:A:128:LYS:HD2	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:204:LYS:HD3	3:A:869:HOH:O	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:HB3	1:A:328:VAL:HG22	1.75	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
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:98:LEU:HD12	1:A:296:MET:HE2	1.85	0.57
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:310:LYS:NZ	3:A:568:HOH:O	2.40	0.54
1:A:104:ILE:HD13	1:A:287:TYR:HB3	1.89	0.54
1:A:127:PRO:HG2	1:A:128:LYS:CE	2.25	0.54
1:A:184:ILE:HA	1:A:198:ASN:OD1	2.08	0.53
1:A:244:GLU:CD	3:A:790:HOH:O	2.51	0.52
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:128:LYS:NZ	3:A:725:HOH:O	2.42	0.52
1:A:127:PRO:CG	1:A:128:LYS:CE	2.86	0.51
1:A:315:LYS:O	1:A:315:LYS:HE3	2.11	0.51
1:A:127:PRO:N	1:A:128:LYS:HE3	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:120:ALA:HA	1:A:133:ASP:OD1	2.14	0.47
1:A:130:TYR:HA	1:A:131:PRO:HD2	1.74	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
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:186:LEU:HD13	1:A:186:LEU:C	2.41	0.45
1:A:4:GLU:CG	1:A:80:TYR:OH	2.63	0.45
1:A:116:LYS:CD	3:A:592:HOH:O	2.64	0.44
1:A:186:LEU:HD22	1:A:186:LEU:HA	1.25	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:11:CYS:CB	1:A:49:LEU:HD21	2.41	0.44
1:A:352:ASP:HA	3:A:844:HOH:O	2.01	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:HG2	1:A:230:ARG:HH11	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:253:PHE:HB3	1:A:256:ASP:HB2	2.01	0.43
1:A:369:LYS:CE	3:A:576:HOH:O	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:O	1:A:187:PRO:C	2.61	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:101:VAL:HG22	1:A:293:ILE:HD13	2.00	0.42
1:A:384:VAL:O	1:A:410:VAL:HA	2.20	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:135:HIS:CD2	1:A:135:HIS:C	2.98	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: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	Interatomic distance (Å)	Clash overlap (Å)
3:A:827:HOH:O	3:A:835:HOH:O[4_647]	2.04	0.16

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	340/440 (77%)	332 (98%)	6 (2%)	2 (1%)	21 9

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%)	358 (94%)	24 (6%)	16 5

All (24) 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	65	ASN
1	A	68	THR
1	A	95	LEU
1	A	98	LEU
1	A	128	LYS
1	A	155	LEU
1	A	164	THR
1	A	174	GLN
1	A	178	ASP
1	A	186	LEU
1	A	189	GLU
1	A	202	LEU
1	A	226	GLU
1	A	244	GLU
1	A	277	MET
1	A	282	LYS
1	A	315	LYS
1	A	327	SER
1	A	410	VAL
1	A	429	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	ASN
1	A	157	GLN
1	A	174	GLN
1	A	193	GLN
1	A	250	ASN
1	A	252	GLN
1	A	255	ASN
1	A	336	GLN
1	A	388	ASN
1	A	430	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

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	440/440 (100%)	-0.40	8 (1%) 67 72	8, 19, 41, 65	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	LEU	5.1
1	A	188	ALA	3.8
1	A	187	PRO	3.5
1	A	427	ASN	3.1
1	A	426	ALA	2.9
1	A	428	GLN	2.3
1	A	424	ASP	2.1
1	A	429	ASP	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	ZN	A	445	1/1	0.99	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.