Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:59 am BST

PDB ID	:	4QMB
Title	:	The structure of inorganic pyrophosphatase from Schistosoma japonicum
Authors	:	Wu, Q.F.
Deposited on	:	2014-06-15
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

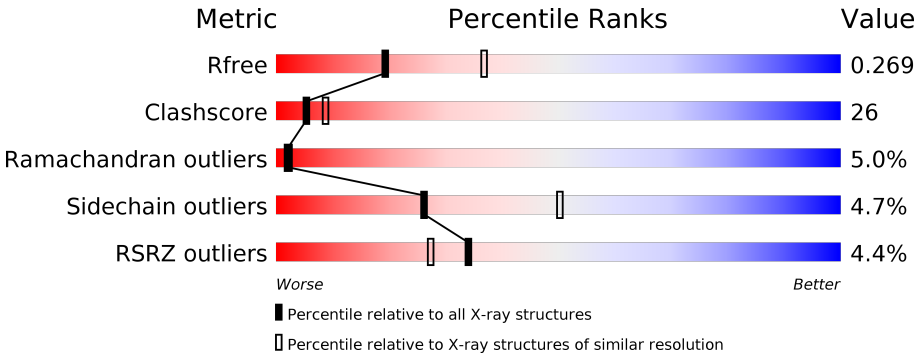
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 >=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 <=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	287	5% 68% 26% 5%
1	B	287	4% 70% 21% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4618 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 SJCHGC07024 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2271	1458	377	424	12			
1	B	283	Total	C	N	O	S	0	0	0
			2259	1450	375	421	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ALA	VAL	ENGINEERED MUTATION	UNP Q5DE13
B	214	ALA	VAL	ENGINEERED MUTATION	UNP Q5DE13

- Molecule 2 is water.

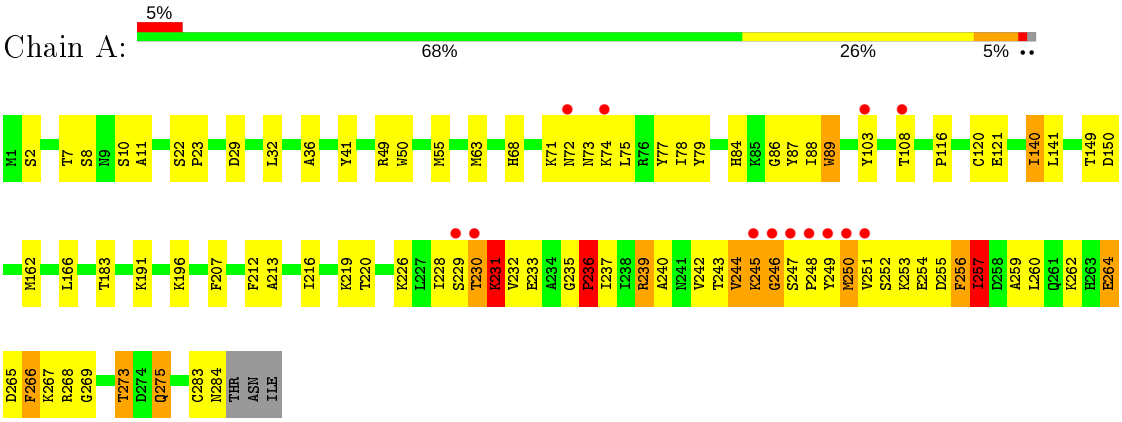
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	50	Total	O	0	0
			50	50		

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 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.

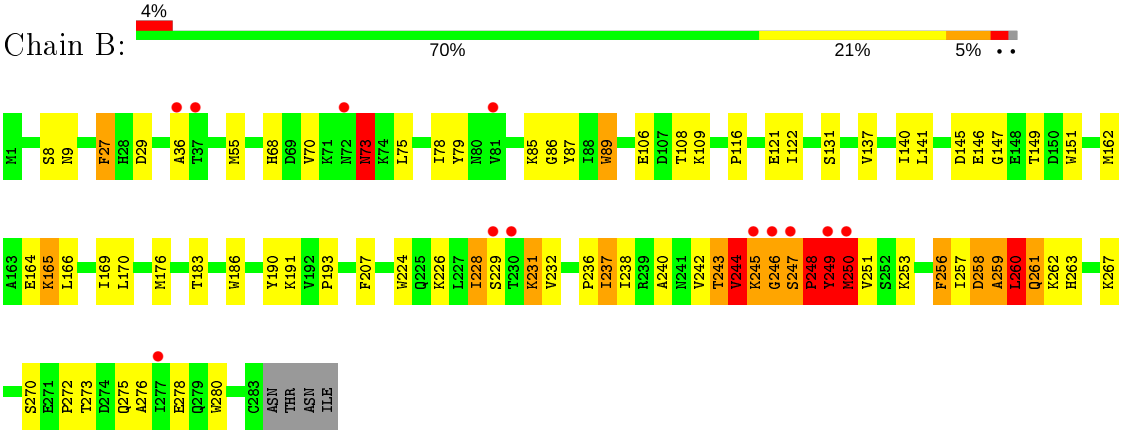
- Molecule 1: SJCHGC07024 protein

Chain A:



- Molecule 1: SJCHGC07024 protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	75.75Å 75.75Å 122.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.88 – 2.60 37.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.88-2.60) 98.1 (37.88-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.36 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202 , 0.263 0.217 , 0.269	Depositor DCC
R_{free} test set	1985 reflections (8.24%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.468 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4618	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.54	0/2336	0.71	2/3168 (0.1%)
1	B	0.53	0/2323	0.69	3/3150 (0.1%)
All	All	0.53	0/4659	0.70	5/6318 (0.1%)

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	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	260	LEU	CA-CB-CG	8.35	134.51	115.30
1	B	248	PRO	N-CA-C	-6.66	94.80	112.10
1	A	231	LYS	CD-CE-NZ	-6.46	96.84	111.70
1	B	243	THR	N-CA-C	-6.33	93.90	111.00
1	A	257	ILE	N-CA-C	-5.31	96.66	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	PRO	Peptide
1	A	244	VAL	Peptide
1	B	244	VAL	Peptide
1	B	249	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	250	MET	Peptide
1	B	261	GLN	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	2271	0	2198	123	0
1	B	2259	0	2195	115	0
2	A	38	0	0	8	0
2	B	50	0	0	1	0
All	All	4618	0	4393	235	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 26.

All (235) 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:236:PRO:O	1:A:237:ILE:HG22	1.16	1.32
1:B:245:LYS:N	1:B:248:PRO:HD2	1.40	1.31
1:B:245:LYS:HG3	1:B:249:TYR:CB	1.60	1.30
1:A:247:SER:HB2	1:A:249:TYR:CD2	1.71	1.24
1:B:244:VAL:C	1:B:248:PRO:HD2	1.60	1.22
1:A:248:PRO:CD	1:A:249:TYR:HA	1.67	1.21
1:A:246:GLY:HA3	1:A:247:SER:OG	1.35	1.20
1:B:247:SER:HA	1:B:249:TYR:HD1	1.06	1.17
1:B:29:ASP:OD1	1:B:243:THR:O	1.61	1.17
1:B:245:LYS:HB2	1:B:249:TYR:HA	1.25	1.16
1:A:247:SER:CB	1:A:249:TYR:HD2	1.58	1.16
1:B:245:LYS:CG	1:B:249:TYR:CB	2.24	1.16
1:A:249:TYR:O	1:A:250:MET:C	1.75	1.15
1:A:247:SER:CB	1:A:249:TYR:CD2	2.30	1.15
1:A:248:PRO:HD2	1:A:249:TYR:CA	1.66	1.14
1:B:245:LYS:HG3	1:B:249:TYR:HB2	1.28	1.13
1:B:243:THR:O	1:B:244:VAL:HB	1.51	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PRO:HB3	1:A:254:GLU:OE1	1.51	1.08
1:B:245:LYS:HA	1:B:246:GLY:C	1.71	1.07
1:A:248:PRO:HD2	1:A:249:TYR:HA	1.16	1.07
1:A:236:PRO:O	1:A:237:ILE:CG2	2.06	1.02
1:B:245:LYS:H	1:B:248:PRO:CD	1.71	1.01
1:B:245:LYS:CG	1:B:249:TYR:HB3	1.89	1.00
1:B:247:SER:O	1:B:249:TYR:CD1	2.13	0.99
1:A:247:SER:C	1:A:249:TYR:HA	1.82	0.99
1:B:245:LYS:HG3	1:B:249:TYR:CA	1.93	0.99
1:B:247:SER:HA	1:B:249:TYR:CD1	1.98	0.98
1:A:249:TYR:O	1:A:251:VAL:N	1.96	0.97
1:A:248:PRO:N	1:A:249:TYR:HA	1.79	0.97
1:B:245:LYS:CB	1:B:249:TYR:HA	1.95	0.97
1:B:245:LYS:HG2	1:B:249:TYR:HB3	1.46	0.96
1:B:247:SER:CA	1:B:249:TYR:HD1	1.80	0.95
1:A:248:PRO:CD	1:A:249:TYR:CA	2.30	0.94
1:B:244:VAL:O	1:B:248:PRO:HD2	1.69	0.92
1:A:236:PRO:C	1:A:237:ILE:HG22	1.89	0.92
1:A:251:VAL:HG12	1:A:253:LYS:H	1.38	0.87
1:B:245:LYS:H	1:B:248:PRO:HD2	1.07	0.85
1:A:247:SER:OG	1:A:249:TYR:CD2	2.30	0.84
1:B:226:LYS:O	1:B:231:LYS:HG2	1.78	0.84
1:A:247:SER:OG	1:A:249:TYR:CE2	2.30	0.83
1:B:247:SER:O	1:B:249:TYR:CG	2.28	0.82
1:B:244:VAL:O	1:B:248:PRO:CG	2.30	0.80
1:A:29:ASP:OD1	1:A:244:VAL:HB	1.80	0.80
1:A:248:PRO:HB2	1:A:251:VAL:H	1.43	0.80
1:B:244:VAL:O	1:B:248:PRO:CD	2.30	0.80
1:B:244:VAL:O	1:B:248:PRO:HB2	1.80	0.79
1:A:242:VAL:HG23	1:A:244:VAL:H	1.49	0.78
1:B:231:LYS:N	1:B:231:LYS:HD3	1.98	0.78
1:B:245:LYS:HB2	1:B:249:TYR:CA	2.13	0.78
1:B:231:LYS:H	1:B:231:LYS:HD3	1.48	0.77
1:B:245:LYS:CG	1:B:249:TYR:CA	2.60	0.77
1:A:236:PRO:C	1:A:237:ILE:CG2	2.52	0.77
1:A:240:ALA:O	1:A:242:VAL:HG12	1.85	0.77
1:A:244:VAL:HA	1:A:245:LYS:HB2	1.65	0.76
1:A:244:VAL:HG22	1:A:245:LYS:HB2	1.67	0.74
1:B:245:LYS:N	1:B:248:PRO:CD	2.30	0.74
1:B:164:GLU:HG3	1:B:165:LYS:HD2	1.70	0.73
1:A:275:GLN:N	2:A:303:HOH:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:NZ	2:A:335:HOH:O	2.17	0.72
1:B:251:VAL:HG12	1:B:253:LYS:H	1.55	0.72
1:B:244:VAL:O	1:B:248:PRO:CB	2.37	0.71
1:B:245:LYS:CG	1:B:249:TYR:HA	2.18	0.71
1:B:106:GLU:O	1:B:109:LYS:NZ	2.23	0.70
1:B:240:ALA:O	1:B:242:VAL:HG12	1.91	0.70
1:A:259:ALA:O	1:A:262:LYS:HG2	1.91	0.70
1:B:245:LYS:HG3	1:B:249:TYR:HA	1.71	0.70
1:B:248:PRO:O	1:B:250:MET:N	2.25	0.70
1:B:242:VAL:HG21	1:B:248:PRO:HB2	1.74	0.69
1:B:8:SER:O	1:B:270:SER:OG	2.07	0.69
1:B:228:ILE:O	1:B:251:VAL:HG13	1.92	0.69
1:B:245:LYS:CG	1:B:249:TYR:HB2	2.06	0.69
1:A:140:ILE:HD11	1:A:212:PHE:HD2	1.58	0.68
1:A:231:LYS:HD3	1:A:233:GLU:OE1	1.94	0.68
1:A:247:SER:C	1:A:249:TYR:CA	2.60	0.68
1:B:242:VAL:HG21	1:B:248:PRO:CB	2.24	0.67
1:B:243:THR:O	1:B:244:VAL:CB	2.29	0.67
1:A:246:GLY:HA3	1:A:247:SER:CB	2.16	0.67
1:B:260:LEU:HG	1:B:261:GLN:OE1	1.94	0.67
1:B:245:LYS:HA	1:B:247:SER:N	2.10	0.66
1:A:268:ARG:NH1	1:A:269:GLY:O	2.29	0.66
1:B:145:ASP:O	1:B:147:GLY:N	2.29	0.66
1:B:78:ILE:HD11	1:B:86:GLY:HA2	1.78	0.65
1:A:228:ILE:O	1:A:251:VAL:HG13	1.97	0.65
1:A:284:ASN:OD1	2:A:333:HOH:O	2.13	0.64
1:A:150:ASP:OD1	2:A:304:HOH:O	2.14	0.64
1:A:244:VAL:HG22	1:A:245:LYS:CB	2.27	0.64
1:B:236:PRO:O	1:B:238:ILE:N	2.30	0.64
1:B:245:LYS:CB	1:B:249:TYR:CA	2.70	0.64
1:B:78:ILE:HG12	1:B:87:TYR:CE1	2.33	0.64
1:A:257:ILE:O	2:A:324:HOH:O	2.15	0.63
1:A:140:ILE:HD11	1:A:212:PHE:CD2	2.33	0.63
1:B:258:ASP:O	1:B:260:LEU:N	2.32	0.63
1:B:55:MET:HE1	1:B:68:HIS:HA	1.79	0.63
1:A:235:GLY:N	1:A:236:PRO:HD2	2.14	0.62
1:A:247:SER:CA	1:A:249:TYR:HA	2.29	0.62
1:A:226:LYS:NZ	2:A:308:HOH:O	2.20	0.61
1:B:244:VAL:HA	1:B:245:LYS:C	2.20	0.61
1:A:244:VAL:CA	1:A:245:LYS:HB2	2.30	0.61
1:A:247:SER:OG	1:A:249:TYR:HE2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:HE1	1:A:68:HIS:HA	1.82	0.60
1:A:248:PRO:HB2	1:A:251:VAL:N	2.14	0.60
1:A:248:PRO:HB2	1:A:251:VAL:HG23	1.82	0.60
1:A:246:GLY:N	1:A:247:SER:O	2.36	0.59
1:B:247:SER:C	1:B:249:TYR:CD1	2.75	0.59
1:B:247:SER:CA	1:B:249:TYR:CD1	2.70	0.59
1:A:78:ILE:HG12	1:A:87:TYR:CE1	2.38	0.58
1:A:78:ILE:HD11	1:A:86:GLY:HA2	1.86	0.58
1:B:8:SER:HB3	1:B:267:LYS:NZ	2.19	0.57
1:B:245:LYS:CA	1:B:246:GLY:C	2.61	0.57
1:A:71:LYS:O	1:A:72:ASN:HB2	2.05	0.56
1:B:248:PRO:HB3	1:B:251:VAL:CG2	2.35	0.56
1:A:229:SER:C	1:A:231:LYS:N	2.59	0.56
1:A:246:GLY:CA	1:A:247:SER:OG	2.30	0.56
1:B:258:ASP:C	1:B:260:LEU:H	2.09	0.56
1:A:247:SER:CA	1:A:249:TYR:HD2	2.18	0.55
1:B:89:TRP:HB3	1:B:121:GLU:O	2.06	0.55
1:A:253:LYS:HE2	2:A:331:HOH:O	2.07	0.55
1:A:256:PHE:CG	1:A:257:ILE:N	2.74	0.55
1:B:244:VAL:O	1:B:248:PRO:HG2	2.07	0.55
1:A:249:TYR:O	1:A:250:MET:O	2.23	0.55
1:A:229:SER:C	1:A:231:LYS:H	2.10	0.54
1:B:122:ILE:HD12	1:B:176:MET:HE1	1.89	0.54
1:A:84:HIS:HD2	2:B:347:HOH:O	1.91	0.54
1:B:229:SER:O	1:B:251:VAL:HA	2.09	0.53
1:B:247:SER:H	1:B:248:PRO:HD3	1.73	0.53
1:B:245:LYS:HG2	1:B:249:TYR:CB	2.15	0.53
1:B:165:LYS:N	1:B:165:LYS:HD2	2.24	0.53
1:A:77:TYR:CZ	1:A:273:THR:HG21	2.44	0.53
1:B:164:GLU:HG3	1:B:165:LYS:CD	2.38	0.53
1:A:68:HIS:ND1	1:A:75:LEU:HD13	2.24	0.52
1:A:229:SER:O	1:A:231:LYS:N	2.42	0.52
1:B:140:ILE:HD11	1:B:151:TRP:HB3	1.91	0.52
1:B:29:ASP:OD1	1:B:244:VAL:HB	2.10	0.52
1:B:244:VAL:C	1:B:248:PRO:CD	2.52	0.52
1:A:247:SER:O	1:A:248:PRO:C	2.49	0.51
1:A:162:MET:HE3	1:A:166:LEU:HD21	1.92	0.51
1:B:244:VAL:HG12	1:B:248:PRO:HG2	1.92	0.51
1:B:248:PRO:C	1:B:250:MET:N	2.63	0.51
1:A:50:TRP:CE3	1:B:85:LYS:HD3	2.46	0.51
1:A:246:GLY:HA3	1:A:247:SER:HG	1.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:N	1:A:248:PRO:HA	2.25	0.50
1:A:63:MET:SD	1:A:259:ALA:HB1	2.51	0.50
1:B:162:MET:HE3	1:B:166:LEU:HD21	1.93	0.50
1:B:258:ASP:C	1:B:260:LEU:N	2.65	0.50
1:A:245:LYS:O	1:A:246:GLY:O	2.30	0.50
1:B:228:ILE:HG22	1:B:229:SER:N	2.27	0.50
1:A:244:VAL:CG2	1:A:245:LYS:HB2	2.38	0.49
1:B:70:VAL:HG12	1:B:75:LEU:HD12	1.95	0.49
1:B:242:VAL:HG11	1:B:251:VAL:HG21	1.93	0.49
1:A:264:GLU:O	1:A:266:PHE:N	2.42	0.49
1:A:244:VAL:O	1:A:248:PRO:O	2.29	0.49
1:A:78:ILE:HD12	1:A:79:TYR:O	2.13	0.49
1:A:23:PRO:HG3	1:A:262:LYS:HD3	1.94	0.49
1:B:79:TYR:CD2	1:B:193:PRO:HG2	2.47	0.49
1:A:8:SER:HB3	1:A:267:LYS:HE2	1.95	0.49
1:A:140:ILE:CD1	1:A:213:ALA:HA	2.43	0.48
1:A:88:ILE:HG13	1:A:89:TRP:CE2	2.48	0.48
1:A:226:LYS:O	1:A:231:LYS:HB2	2.13	0.48
1:B:169:ILE:HG23	1:B:170:LEU:HD12	1.95	0.48
1:B:261:GLN:HA	1:B:263:HIS:H	1.78	0.48
1:A:141:LEU:HB2	1:A:207:PHE:CE1	2.49	0.48
1:A:246:GLY:CA	1:A:247:SER:C	2.82	0.48
1:A:246:GLY:CA	1:A:247:SER:O	2.62	0.48
1:A:103:TYR:HB2	2:A:321:HOH:O	2.14	0.47
1:A:246:GLY:HA3	1:A:247:SER:O	2.14	0.47
1:B:236:PRO:C	1:B:238:ILE:H	2.15	0.47
1:B:245:LYS:H	1:B:247:SER:N	2.13	0.47
1:A:10:SER:OG	1:A:11:ALA:N	2.48	0.47
1:A:246:GLY:N	1:A:247:SER:C	2.67	0.47
1:B:8:SER:HB3	1:B:267:LYS:HZ2	1.80	0.47
1:B:89:TRP:CD1	1:B:122:ILE:HG22	2.50	0.47
1:B:191:LYS:HD3	1:B:191:LYS:HA	1.81	0.46
1:A:89:TRP:CZ2	1:A:183:THR:HG23	2.50	0.46
1:B:108:THR:HG21	1:B:149:THR:HG23	1.98	0.46
1:B:275:GLN:HG2	1:B:276:ALA:H	1.81	0.46
1:B:247:SER:H	1:B:248:PRO:CD	2.29	0.45
1:B:228:ILE:HG23	1:B:251:VAL:HG22	1.97	0.45
1:A:216:ILE:O	1:A:220:THR:HG23	2.17	0.45
1:A:251:VAL:HB	1:A:254:GLU:N	2.32	0.45
1:B:141:LEU:HB2	1:B:207:PHE:CE1	2.51	0.45
1:A:230:THR:HA	1:A:252:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:SER:C	1:A:249:TYR:HD2	2.19	0.45
1:A:50:TRP:CD2	1:B:85:LYS:HD3	2.51	0.45
1:A:251:VAL:HB	1:A:254:GLU:H	1.80	0.45
1:B:261:GLN:C	1:B:263:HIS:N	2.70	0.44
1:A:244:VAL:HG13	1:A:245:LYS:N	2.32	0.44
1:B:73:ASN:N	1:B:73:ASN:OD1	2.51	0.44
1:A:247:SER:O	1:A:249:TYR:CD2	2.70	0.44
1:A:89:TRP:HB3	1:A:121:GLU:O	2.17	0.44
1:B:256:PHE:HA	1:B:257:ILE:HA	1.47	0.44
1:A:219:LYS:HD3	1:A:219:LYS:HA	1.82	0.44
1:A:247:SER:HA	1:A:249:TYR:HA	1.97	0.44
1:A:49:ARG:NH2	1:B:278:GLU:O	2.51	0.44
1:A:233:GLU:OE1	1:A:233:GLU:N	2.50	0.44
1:B:186:TRP:O	1:B:190:TYR:HB3	2.17	0.44
1:B:242:VAL:HG21	1:B:248:PRO:HB3	1.99	0.43
1:A:78:ILE:HD11	1:A:86:GLY:CA	2.47	0.43
1:B:242:VAL:CG2	1:B:248:PRO:HB2	2.46	0.43
1:A:22:SER:HA	1:A:23:PRO:HD2	1.88	0.43
1:A:7:THR:O	1:A:10:SER:HB3	2.18	0.43
1:A:63:MET:CE	1:A:262:LYS:HB3	2.48	0.43
1:A:247:SER:CB	1:A:249:TYR:CE2	2.90	0.42
1:B:258:ASP:CG	1:B:259:ALA:N	2.71	0.42
1:A:140:ILE:HD13	1:A:213:ALA:HA	2.01	0.42
1:A:108:THR:HG21	1:A:149:THR:HG23	2.00	0.42
1:A:89:TRP:HZ2	1:A:183:THR:HG1	1.67	0.42
1:B:89:TRP:CZ2	1:B:183:THR:HG23	2.54	0.42
1:B:245:LYS:N	1:B:247:SER:N	2.68	0.42
1:A:191:LYS:HE3	1:A:196:LYS:HD3	2.02	0.42
1:A:242:VAL:HG23	1:A:243:THR:N	2.34	0.42
1:A:140:ILE:HG21	1:A:140:ILE:HD13	1.79	0.41
1:A:245:LYS:HG2	1:A:245:LYS:O	2.19	0.41
1:A:268:ARG:HD2	1:A:269:GLY:O	2.20	0.41
1:B:226:LYS:HA	1:B:231:LYS:HE2	2.03	0.41
1:B:261:GLN:C	1:B:263:HIS:H	2.24	0.41
1:A:89:TRP:CG	1:A:120:CYS:HB3	2.55	0.41
1:B:27:PHE:CE1	1:B:116:PRO:HG3	2.56	0.41
1:B:78:ILE:HD12	1:B:79:TYR:O	2.20	0.41
1:B:78:ILE:CD1	1:B:86:GLY:HA2	2.48	0.41
1:A:77:TYR:OH	1:A:273:THR:HG21	2.20	0.41
1:B:89:TRP:HZ2	1:B:183:THR:HG1	1.66	0.41
1:A:74:LYS:HB3	1:A:74:LYS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:HD11	1:B:86:GLY:CA	2.46	0.41
1:A:235:GLY:N	1:A:236:PRO:CD	2.81	0.41
1:A:244:VAL:C	1:A:248:PRO:HA	2.41	0.41
1:A:32:LEU:HD11	1:A:41:TYR:HD2	1.86	0.41
1:B:237:ILE:HG12	1:B:237:ILE:O	2.20	0.41
1:A:246:GLY:CA	1:A:247:SER:CB	2.91	0.41
1:A:260:LEU:C	1:A:262:LYS:H	2.24	0.40
1:A:249:TYR:C	1:A:251:VAL:N	2.67	0.40
1:B:224:TRP:CZ2	1:B:228:ILE:HG13	2.57	0.40
1:B:247:SER:N	1:B:248:PRO:CD	2.84	0.40
1:B:9:ASN:ND2	1:B:272:PRO:HA	2.37	0.40
1:B:8:SER:HB3	1:B:267:LYS:HZ1	1.85	0.40
1:A:239:ARG:HA	1:A:239:ARG:HD2	1.55	0.40

There are no symmetry-related clashes.

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	282/287 (98%)	255 (90%)	16 (6%)	11 (4%)	3 4
1	B	281/287 (98%)	242 (86%)	22 (8%)	17 (6%)	1 1
All	All	563/574 (98%)	497 (88%)	38 (7%)	28 (5%)	2 2

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	PRO
1	A	245	LYS
1	A	250	MET
1	A	256	PHE
1	A	265	ASP

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Mol	Chain	Res	Type
1	A	275	GLN
1	B	73	ASN
1	B	146	GLU
1	B	237	ILE
1	B	248	PRO
1	B	249	TYR
1	B	250	MET
1	B	258	ASP
1	B	259	ALA
1	A	246	GLY
1	A	266	PHE
1	B	231	LYS
1	B	244	VAL
1	B	256	PHE
1	B	262	LYS
1	A	73	ASN
1	A	230	THR
1	B	36	ALA
1	B	273	THR
1	B	247	SER
1	B	260	LEU
1	A	36	ALA
1	B	246	GLY

5.3.2 Protein sidechains (i)

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	245/251 (98%)	233 (95%)	12 (5%)	25 48
1	B	244/251 (97%)	233 (96%)	11 (4%)	27 52
All	All	489/502 (97%)	466 (95%)	23 (5%)	26 50

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	89	TRP
1	A	116	PRO
1	A	140	ILE
1	A	231	LYS
1	A	232	VAL
1	A	239	ARG
1	A	255	ASP
1	A	257	ILE
1	A	264	GLU
1	A	273	THR
1	A	283	CYS
1	B	27	PHE
1	B	73	ASN
1	B	89	TRP
1	B	131	SER
1	B	137	VAL
1	B	165	LYS
1	B	228	ILE
1	B	232	VAL
1	B	244	VAL
1	B	245	LYS
1	B	280	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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^{th} 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	284/287 (98%)	0.29	13 (4%)	32	26	24, 50, 104, 129	0
1	B	283/287 (98%)	0.34	12 (4%)	36	29	24, 49, 100, 134	0
All	All	567/574 (98%)	0.31	25 (4%)	34	27	24, 50, 103, 134	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	10.5
1	A	230	THR	8.1
1	B	247	SER	7.4
1	B	72	ASN	7.1
1	A	108	THR	6.7
1	A	247	SER	5.6
1	A	246	GLY	5.6
1	B	250	MET	4.6
1	A	249	TYR	4.3
1	B	37	THR	4.3
1	A	245	LYS	4.2
1	B	229	SER	4.0
1	B	249	TYR	3.7
1	A	72	ASN	3.6
1	B	230	THR	3.6
1	B	245	LYS	3.5
1	B	81	VAL	3.1
1	A	74	LYS	2.8
1	A	251	VAL	2.5
1	A	103	TYR	2.5
1	A	229	SER	2.4
1	A	250	MET	2.3
1	A	248	PRO	2.2
1	B	277	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	36	ALA	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 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.