Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:12 PM EDT

PDB ID	:	3QRV
Title	:	Crystal structure of plasmepsin I (PMI) from Plasmodium falciparum
Authors	:	Bhaumik, P.; Gustchina, A.; Wlodawer, A.
Deposited on	:	2011-02-18
Resolution	:	2.40 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:

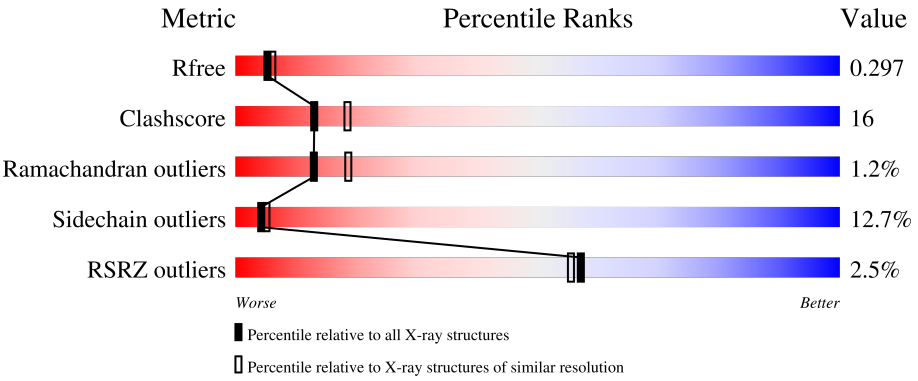
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	336	2% 60% 29% 7%
1	B	336	2% 62% 29% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5379 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 Plasmepsin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2571	1673	398	493	7			
1	B	329	Total	C	N	O	S	0	0	0
			2620	1703	406	503	8			

- Molecule 2 is water.

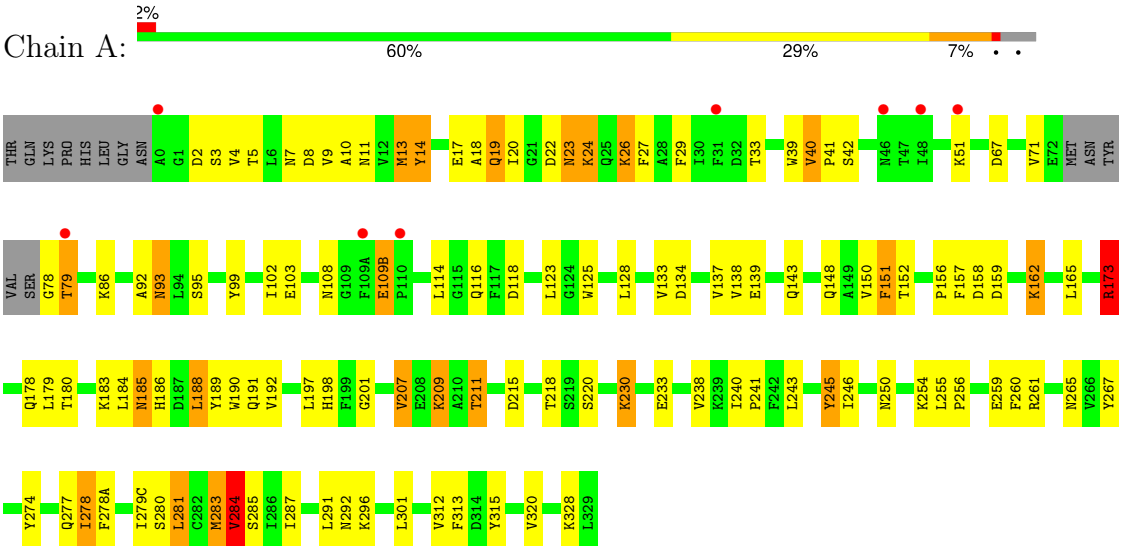
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	107	Total	O	0	0
			107	107		
2	B	81	Total	O	0	0
			81	81		

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.

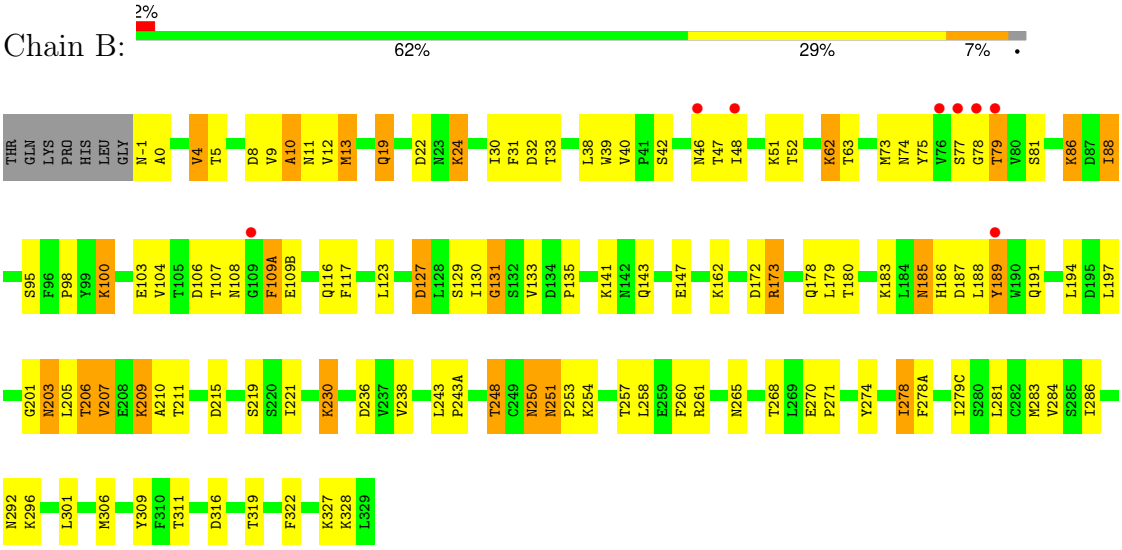
• Molecule 1: Plasmepsin-1

Chain A:



• Molecule 1: Plasmepsin-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.17Å 93.39Å 108.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.40) 99.6 (29.93-2.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.207 , 0.283 0.220 , 0.297	Depositor DCC
R_{free} test set	1465 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5379	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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	1.13	5/2635 (0.2%)	1.04	5/3578 (0.1%)
1	B	1.13	2/2686 (0.1%)	1.10	7/3649 (0.2%)
All	All	1.13	7/5321 (0.1%)	1.07	12/7227 (0.2%)

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	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	VAL	CB-CG1	-7.23	1.37	1.52
1	A	14	TYR	CD2-CE2	6.51	1.49	1.39
1	A	245	TYR	CD1-CE1	6.39	1.49	1.39
1	B	147	GLU	CD-OE1	6.01	1.32	1.25
1	B	127	ASP	CB-CG	-5.59	1.40	1.51
1	A	151	PHE	CE2-CZ	5.19	1.47	1.37
1	A	274	TYR	CD1-CE1	5.10	1.47	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	172	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	320	VAL	CB-CA-C	-6.79	98.50	111.40
1	B	32	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	230	LYS	CD-CE-NZ	5.97	125.43	111.70
1	A	40	VAL	CB-CA-C	-5.95	100.09	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254	LYS	CD-CE-NZ	-5.92	98.08	111.70
1	B	131	GLY	N-CA-C	-5.86	98.45	113.10
1	B	172	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	173	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	306	MET	CG-SD-CE	5.25	108.59	100.20
1	B	127	ASP	N-CA-CB	-5.18	101.27	110.60
1	A	157	PHE	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109(B)	GLU	Peptide
1	B	130	ILE	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	2571	0	2507	84	0
1	B	2620	0	2552	87	0
2	A	107	0	0	10	0
2	B	81	0	0	14	0
All	All	5379	0	5059	168	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 16.

All (168) 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:B:13:MET:HE1	1:B:116:GLN:H	1.12	1.14
1:A:211:THR:HG22	2:A:367:HOH:O	1.62	0.99
1:B:13:MET:CE	1:B:116:GLN:H	1.80	0.95
1:B:13:MET:HE1	1:B:116:GLN:N	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MET:HE1	1:A:116:GLN:H	1.38	0.87
1:B:116:GLN:HA	2:B:400:HOH:O	1.75	0.86
1:B:250:ASN:ND2	1:B:250:ASN:H	1.75	0.85
1:B:250:ASN:CG	2:B:358:HOH:O	2.17	0.83
1:A:23:ASN:HB2	2:A:373:HOH:O	1.77	0.83
1:A:209:LYS:HE2	2:A:334:HOH:O	1.77	0.83
1:B:81:SER:OG	1:B:106:ASP:HB3	1.78	0.82
1:A:278:ILE:HD13	1:A:283:MET:HB3	1.63	0.79
1:B:207:VAL:HG22	1:B:210:ALA:HB2	1.65	0.78
1:B:250:ASN:H	1:B:250:ASN:HD22	1.30	0.77
1:B:77:SER:HB3	1:B:109(A):PHE:CE1	2.20	0.76
1:B:250:ASN:HD22	1:B:250:ASN:N	1.86	0.74
1:B:185:ASN:HD22	1:B:186:HIS:N	1.88	0.72
1:A:9:VAL:HG11	1:A:13:MET:HE2	1.71	0.72
1:A:13:MET:CE	1:A:116:GLN:H	2.04	0.70
1:B:205:LEU:HD21	1:B:230:LYS:HD3	1.73	0.69
1:A:218:THR:HG22	1:A:220:SER:H	1.56	0.69
1:B:42:SER:HB2	1:B:103:GLU:HB3	1.74	0.69
1:A:279(C):ILE:HG13	1:A:280:SER:H	1.56	0.68
1:B:12:VAL:O	1:B:219:SER:HB3	1.93	0.68
1:A:189:TYR:H	1:A:191:GLN:HE21	1.41	0.67
1:A:78:GLY:O	1:A:79:THR:HG22	1.94	0.66
1:A:22:ASP:N	1:A:22:ASP:OD1	2.27	0.65
1:A:5:THR:CG2	1:A:162:LYS:HG2	2.27	0.65
1:B:131:GLY:HA2	2:B:357:HOH:O	1.97	0.64
1:A:197:LEU:HD22	1:A:260:PHE:HD1	1.63	0.64
1:A:279(C):ILE:HG13	1:A:280:SER:N	2.13	0.64
1:B:109(B):GLU:HA	1:B:109(B):GLU:OE1	1.97	0.63
1:B:180:THR:CG2	1:B:265:ASN:ND2	2.62	0.62
1:A:137:VAL:HG23	2:A:336:HOH:O	1.99	0.62
1:A:71:VAL:HG21	1:A:102:ILE:HD13	1.82	0.62
1:B:127:ASP:OD2	1:B:129:SER:HB2	2.00	0.62
1:B:73:MET:HB2	2:B:405:HOH:O	2.00	0.61
1:A:139:GLU:O	1:A:143:GLN:HG3	2.01	0.61
1:A:18:ALA:HB3	1:A:29:PHE:CE1	2.37	0.60
1:A:240:ILE:HD11	1:A:246:ILE:HD13	1.82	0.60
1:B:131:GLY:CA	2:B:357:HOH:O	2.51	0.59
1:A:240:ILE:HD11	1:A:246:ILE:CD1	2.33	0.58
1:A:240:ILE:O	1:A:241:PRO:C	2.39	0.58
1:A:279(C):ILE:CG1	1:A:280:SER:N	2.65	0.58
1:B:311:THR:HG22	1:B:322:PHE:CD1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:MET:HE1	1:A:116:GLN:N	2.14	0.58
1:A:152:THR:HG22	1:A:312:VAL:HG22	1.86	0.58
1:A:173:ARG:HD3	2:A:419:HOH:O	2.03	0.58
1:A:278:ILE:HD11	1:A:283:MET:HE2	1.86	0.57
1:A:180:THR:HG23	1:A:265:ASN:CG	2.25	0.57
1:B:77:SER:HB3	1:B:109(A):PHE:HE1	1.65	0.57
1:B:31:PHE:HB3	1:B:123:LEU:HD11	1.85	0.57
1:B:62:LYS:O	1:B:62:LYS:HG2	2.05	0.57
1:A:245:TYR:HB2	1:A:284:VAL:HG13	1.86	0.57
1:B:207:VAL:CG2	1:B:210:ALA:HB2	2.35	0.57
1:B:88:ILE:HD11	1:B:95:SER:HB3	1.86	0.56
1:B:186:HIS:CD2	1:B:187:ASP:H	2.24	0.56
1:B:278:ILE:HG22	1:B:281:LEU:HD23	1.87	0.56
1:A:22:ASP:C	1:A:24:LYS:H	2.09	0.56
1:A:10:ALA:O	1:A:11:ASN:HB2	2.05	0.56
1:B:8:ASP:OD2	1:B:11:ASN:ND2	2.39	0.56
1:B:271:PRO:HA	1:B:274:TYR:CE2	2.41	0.56
1:B:258:LEU:O	1:B:268:THR:HA	2.06	0.56
1:A:188:LEU:HB3	1:A:191:GLN:NE2	2.21	0.56
1:B:5:THR:CG2	1:B:162:LYS:HG2	2.36	0.55
1:A:197:LEU:HB2	1:A:207:VAL:HG13	1.88	0.55
1:A:197:LEU:HD22	1:A:260:PHE:CD1	2.41	0.55
1:B:189:TYR:CD2	1:B:189:TYR:N	2.74	0.55
1:B:180:THR:HG23	1:B:265:ASN:ND2	2.23	0.54
1:B:185:ASN:HD22	1:B:186:HIS:H	1.54	0.54
1:B:186:HIS:CD2	1:B:187:ASP:N	2.75	0.54
1:A:292:ASN:N	2:A:423:HOH:O	2.40	0.54
1:B:248:THR:HG23	2:B:358:HOH:O	2.07	0.54
1:A:51:LYS:HB2	2:A:341:HOH:O	2.07	0.54
1:B:98:PRO:HD2	1:B:143:GLN:HE22	1.72	0.54
1:B:86:LYS:HD2	1:B:100:LYS:HG3	1.90	0.54
1:A:278:ILE:HD11	1:A:283:MET:CE	2.37	0.54
1:B:48:ILE:O	1:B:51:LYS:HB2	2.08	0.54
1:A:133:VAL:HG12	1:A:134:ASP:O	2.08	0.54
1:B:221:ILE:O	1:B:286:ILE:HA	2.08	0.54
1:A:8:ASP:HB2	1:A:14:TYR:CE1	2.43	0.53
1:B:278(A):PHE:HB3	1:B:281:LEU:HB3	1.89	0.53
1:A:180:THR:CG2	1:A:265:ASN:CG	2.77	0.53
1:B:0:ALA:HA	2:B:392:HOH:O	2.09	0.53
1:B:33:THR:OG1	1:B:215:ASP:HA	2.09	0.53
1:A:128:LEU:HD13	1:A:188:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:HD22	1:A:186:HIS:N	2.07	0.52
1:B:46:ASN:HB2	2:B:391:HOH:O	2.09	0.52
1:B:141:LYS:HE2	1:B:316:ASP:OD2	2.09	0.52
1:B:251:ASN:ND2	1:B:254:LYS:H	2.07	0.52
1:A:17:GLU:OE1	1:A:26:LYS:HD2	2.10	0.52
1:A:188:LEU:HD22	1:A:189:TYR:CD2	2.45	0.52
1:B:236:ASP:OD2	1:B:254:LYS:HE3	2.09	0.51
1:A:138:VAL:O	1:A:139:GLU:C	2.49	0.51
1:B:-1:ASN:N	2:B:342:HOH:O	2.34	0.51
1:B:81:SER:HG	1:B:106:ASP:HB3	1.76	0.51
1:B:19:GLN:HE21	1:B:24:LYS:HG2	1.76	0.51
1:B:135:PRO:HB2	2:B:372:HOH:O	2.10	0.51
1:B:251:ASN:HD22	1:B:253:PRO:HD2	1.77	0.50
1:A:198:HIS:HB3	1:A:259:GLU:HB2	1.94	0.49
1:A:67:ASP:C	1:A:67:ASP:OD1	2.51	0.48
1:A:220:SER:OG	1:A:287:ILE:HG12	2.14	0.48
1:A:99:TYR:OH	2:A:293:HOH:O	2.20	0.48
1:B:271:PRO:HA	1:B:274:TYR:CZ	2.49	0.48
1:A:9:VAL:HG13	1:A:9:VAL:O	2.14	0.48
1:A:180:THR:HG22	1:A:267:TYR:OH	2.14	0.48
1:B:278:ILE:CG2	1:B:281:LEU:HD23	2.43	0.48
1:A:19:GLN:HB3	1:A:24:LYS:HG3	1.97	0.47
1:B:180:THR:HG21	1:B:265:ASN:ND2	2.29	0.47
1:A:220:SER:HB2	1:A:285:SER:O	2.15	0.47
1:B:48:ILE:HA	1:B:51:LYS:HD2	1.96	0.47
1:B:292:ASN:HA	2:B:384:HOH:O	2.13	0.47
1:B:278:ILE:HD13	1:B:283:MET:HG2	1.97	0.46
1:B:104:VAL:HG11	1:B:107:THR:HG22	1.95	0.46
1:B:189:TYR:HD2	1:B:189:TYR:H	1.63	0.46
1:A:20:ILE:HD12	1:A:27:PHE:CE1	2.51	0.46
1:A:188:LEU:HB3	1:A:189:TYR:H	1.50	0.46
1:A:33:THR:OG1	1:A:215:ASP:HA	2.16	0.46
1:B:311:THR:HG22	1:B:322:PHE:HD1	1.79	0.46
1:A:18:ALA:HB3	1:A:29:PHE:CD1	2.51	0.45
1:A:42:SER:HB2	1:A:103:GLU:HB3	1.98	0.45
1:A:2:ASP:HB3	1:A:92:ALA:HB1	1.99	0.45
1:A:7:ASN:O	1:A:14:TYR:HA	2.17	0.45
1:A:22:ASP:C	1:A:24:LYS:N	2.68	0.45
1:B:75:TYR:N	1:B:78:GLY:O	2.48	0.45
1:B:309:TYR:O	1:B:311:THR:HG23	2.17	0.45
1:A:255:LEU:HA	1:A:256:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TYR:CE1	1:A:156:PRO:HD2	2.52	0.44
1:B:4:VAL:O	1:B:4:VAL:CG2	2.64	0.44
1:B:251:ASN:HD22	1:B:253:PRO:CD	2.30	0.44
1:A:9:VAL:HG11	1:A:13:MET:CE	2.45	0.44
1:A:148:GLN:HB2	1:A:150:VAL:HG12	1.98	0.44
1:A:278(A):PHE:HB3	1:A:281:LEU:HB2	1.98	0.44
1:B:189:TYR:N	1:B:189:TYR:HD2	2.15	0.44
1:B:203:ASN:N	2:B:341:HOH:O	2.36	0.43
1:A:3:SER:HA	1:A:165:LEU:O	2.17	0.43
1:A:180:THR:HG23	1:A:265:ASN:ND2	2.32	0.43
1:A:125:TRP:HB3	2:A:372:HOH:O	2.19	0.43
1:B:201:GLY:HA3	2:B:341:HOH:O	2.18	0.43
1:A:279(C):ILE:HG22	1:B:279(C):ILE:HG12	2.00	0.43
1:B:186:HIS:HD2	1:B:187:ASP:N	2.15	0.43
1:B:205:LEU:HD11	1:B:230:LYS:HB3	2.01	0.42
1:A:283:MET:O	1:A:283:MET:HG3	2.19	0.42
1:B:38:LEU:HD23	1:B:39:TRP:N	2.35	0.42
1:A:291:LEU:HA	2:A:423:HOH:O	2.20	0.42
1:A:184:LEU:HA	1:A:191:GLN:O	2.18	0.42
1:B:328:LYS:HB2	2:B:385:HOH:O	2.19	0.42
1:A:198:HIS:CD2	1:A:201:GLY:O	2.73	0.41
1:A:151:PHE:CE1	1:A:313:PHE:CD1	3.08	0.41
1:B:30:ILE:HG12	1:B:117:PHE:CD1	2.55	0.41
1:B:74:ASN:OD1	1:B:79:THR:HG23	2.20	0.41
1:A:41:PRO:HD3	1:A:118:ASP:O	2.19	0.41
1:A:108:ASN:HB3	1:B:108:ASN:O	2.20	0.41
1:B:194:LEU:HD13	1:B:260:PHE:HB3	2.03	0.41
1:A:17:GLU:CD	1:A:26:LYS:HD2	2.41	0.41
1:B:10:ALA:O	1:B:11:ASN:HB2	2.21	0.41
1:A:190:TRP:HZ2	1:A:315:TYR:CZ	2.39	0.41
1:A:238:VAL:O	1:A:245:TYR:HA	2.21	0.41
1:A:243:LEU:HD22	1:B:243:LEU:HD22	2.03	0.41
1:A:277:GLN:O	1:A:278:ILE:HD12	2.20	0.41
1:B:209:LYS:HE3	1:B:209:LYS:HA	2.03	0.41
1:B:243:LEU:HA	1:B:243(A):PRO:HD2	1.80	0.40
1:B:197:LEU:O	1:B:206:THR:HA	2.21	0.40
1:B:327:LYS:HD2	1:B:327:LYS:HA	1.81	0.40
1:A:158:ASP:C	1:A:158:ASP:OD2	2.60	0.40
1:B:221:ILE:HB	1:B:286:ILE:HG12	2.03	0.40
1:A:123:LEU:HA	1:A:123:LEU:HD23	1.71	0.40
1:B:257:THR:HG23	1:B:270:GLU:HG3	2.04	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	319/336 (95%)	283 (89%)	30 (9%)	6 (2%)	8 10
1	B	327/336 (97%)	306 (94%)	19 (6%)	2 (1%)	25 36
All	All	646/672 (96%)	589 (91%)	49 (8%)	8 (1%)	13 19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	93	ASN
1	A	109(B)	GLU
1	B	47	THR
1	A	173	ARG
1	B	10	ALA
1	A	188	LEU
1	A	23	ASN

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	284/296 (96%)	251 (88%)	33 (12%)	5 7
1	B	290/296 (98%)	250 (86%)	40 (14%)	3 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	574/592 (97%)	501 (87%)	73 (13%)	4 5

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	13	MET
1	A	19	GLN
1	A	24	LYS
1	A	26	LYS
1	A	39	TRP
1	A	40	VAL
1	A	86	LYS
1	A	93	ASN
1	A	95	SER
1	A	114	LEU
1	A	159	ASP
1	A	162	LYS
1	A	173	ARG
1	A	178	GLN
1	A	179	LEU
1	A	183	LYS
1	A	185	ASN
1	A	192	VAL
1	A	207	VAL
1	A	209	LYS
1	A	211	THR
1	A	230	LYS
1	A	233	GLU
1	A	250	ASN
1	A	261	ARG
1	A	278	ILE
1	A	281	LEU
1	A	283	MET
1	A	284	VAL
1	A	296	LYS
1	A	301	LEU
1	A	328	LYS
1	B	4	VAL
1	B	9	VAL
1	B	13	MET
1	B	19	GLN

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Mol	Chain	Res	Type
1	B	22	ASP
1	B	24	LYS
1	B	40	VAL
1	B	52	THR
1	B	62	LYS
1	B	63	THR
1	B	79	THR
1	B	86	LYS
1	B	88	ILE
1	B	100	LYS
1	B	109(A)	PHE
1	B	133	VAL
1	B	173	ARG
1	B	178	GLN
1	B	179	LEU
1	B	183	LYS
1	B	185	ASN
1	B	188	LEU
1	B	189	TYR
1	B	191	GLN
1	B	203	ASN
1	B	206	THR
1	B	207	VAL
1	B	209	LYS
1	B	211	THR
1	B	230	LYS
1	B	238	VAL
1	B	248	THR
1	B	250	ASN
1	B	251	ASN
1	B	261	ARG
1	B	278	ILE
1	B	284	VAL
1	B	296	LYS
1	B	301	LEU
1	B	319	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	108	ASN
1	A	116	GLN
1	A	143	GLN
1	A	185	ASN
1	A	191	GLN
1	A	203	ASN
1	B	11	ASN
1	B	19	GLN
1	B	116	GLN
1	B	143	GLN
1	B	185	ASN
1	B	186	HIS
1	B	203	ASN
1	B	250	ASN
1	B	251	ASN
1	B	265	ASN
1	B	292	ASN
1	B	297	ASN

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 monosaccharides 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 (i)

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	323/336 (96%)	-0.13	8 (2%)	57	55	22, 38, 74, 91	0
1	B	329/336 (97%)	-0.10	8 (2%)	59	57	23, 39, 70, 87	0
All	All	652/672 (97%)	-0.12	16 (2%)	57	55	22, 39, 73, 91	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	ALA	5.0
1	B	77	SER	4.4
1	B	189	TYR	4.0
1	B	109	GLY	3.7
1	A	109(A)	PHE	3.5
1	B	78	GLY	3.5
1	A	48	ILE	3.3
1	B	76	VAL	3.0
1	A	51	LYS	2.7
1	B	46	ASN	2.6
1	B	48	ILE	2.5
1	B	79	THR	2.5
1	A	31	PHE	2.4
1	A	110	PRO	2.2
1	A	46	ASN	2.1
1	A	79	THR	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 (i)

There are no monosaccharides 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.