



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:21 am GMT

PDB ID : 3MMI  
Title : Crystal structure of the globular tail of Myo4p  
Authors : Heuck, A.; Niessing, D.  
Deposited on : 2010-04-19  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

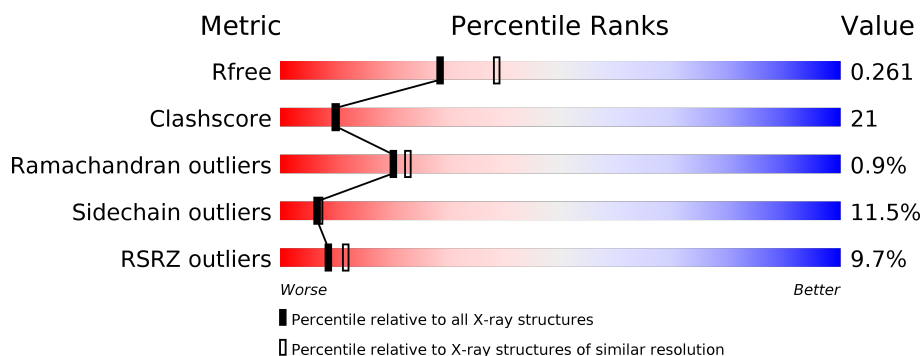
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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. 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	386	<div> <div>9%</div> <div>55%</div> <div>23%</div> <div>5% •</div> <div>16%</div> </div>
1	B	386	<div> <div>8%</div> <div>52%</div> <div>29%</div> <div>8% •</div> <div>10%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5623 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 Myosin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	115	0	0
			2651	1736	427	476	12			
1	B	346	Total	C	N	O	S	172	0	0
			2802	1833	453	504	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1086	GLY	-	EXPRESSION TAG	UNP P32492
A	1087	PRO	-	EXPRESSION TAG	UNP P32492
A	1088	LEU	-	EXPRESSION TAG	UNP P32492
A	1089	GLY	-	EXPRESSION TAG	UNP P32492
A	1090	SER	-	EXPRESSION TAG	UNP P32492
B	1086	GLY	-	EXPRESSION TAG	UNP P32492
B	1087	PRO	-	EXPRESSION TAG	UNP P32492
B	1088	LEU	-	EXPRESSION TAG	UNP P32492
B	1089	GLY	-	EXPRESSION TAG	UNP P32492
B	1090	SER	-	EXPRESSION TAG	UNP P32492

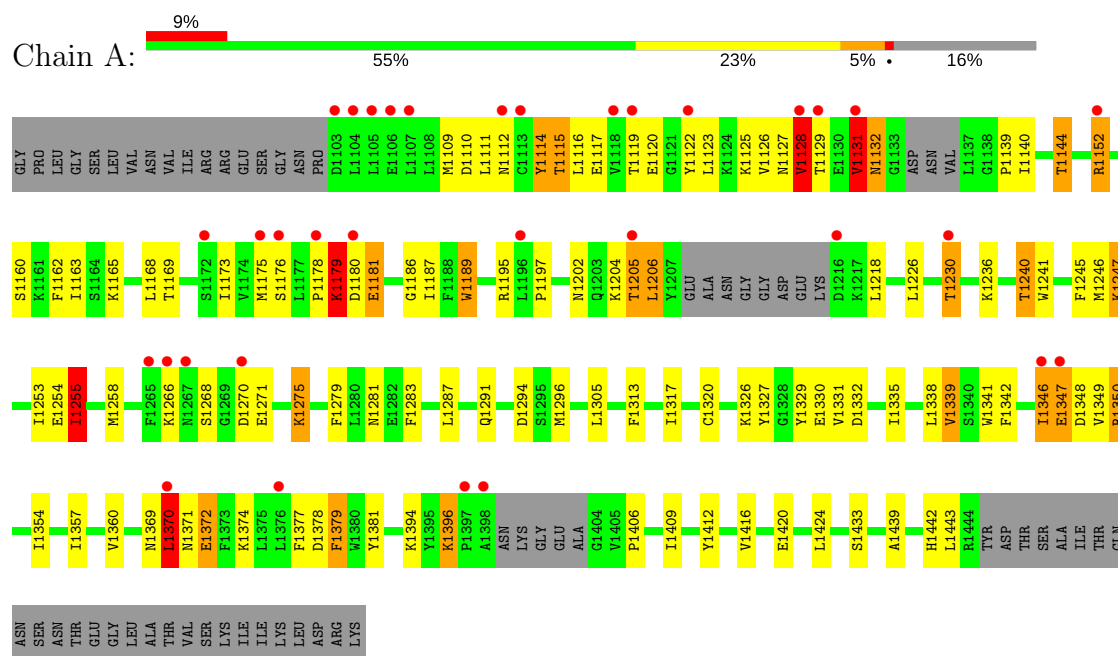
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	90	Total	O	0	0
			90	90		

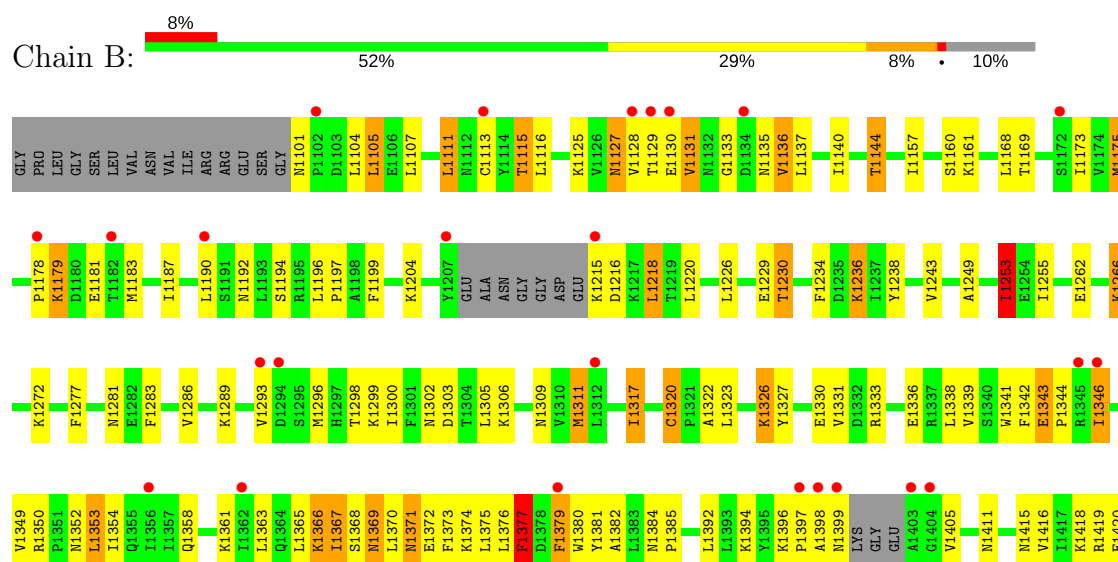
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Myosin-4



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.48Å 120.99Å 157.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.51 – 2.30 29.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.51-2.30) 98.1 (29.57-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.254 , 0.287 0.236 , 0.261	Depositor DCC
$R_{free}$ test set	1855 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

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	1.34	19/2702 (0.7%)	1.10	8/3654 (0.2%)
1	B	1.38	18/2855 (0.6%)	1.08	11/3862 (0.3%)
All	All	1.36	37/5557 (0.7%)	1.09	19/7516 (0.3%)

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	B	0	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1336	GLU	CB-CG	-12.17	1.29	1.52
1	A	1117	GLU	CB-CG	-10.34	1.32	1.52
1	B	1262	GLU	CG-CD	8.90	1.65	1.51
1	B	1125	LYS	CA-CB	-8.86	1.34	1.53
1	A	1271	GLU	CG-CD	7.43	1.63	1.51
1	A	1347	GLU	CB-CG	7.02	1.65	1.52
1	A	1350	ARG	CG-CD	-6.84	1.34	1.51
1	B	1368	SER	CB-OG	6.73	1.51	1.42
1	B	1289	LYS	CE-NZ	-6.69	1.32	1.49
1	A	1416	VAL	CA-CB	6.52	1.68	1.54
1	B	1468	LEU	C-O	6.43	1.35	1.23
1	A	1247	LYS	CG-CD	6.40	1.74	1.52
1	A	1433	SER	CB-OG	-6.31	1.34	1.42
1	B	1416	VAL	CA-CB	6.17	1.67	1.54
1	B	1234	PHE	CE2-CZ	6.08	1.48	1.37
1	A	1329	TYR	CD2-CE2	5.77	1.48	1.39
1	A	1313	PHE	CE1-CZ	5.71	1.48	1.37
1	B	1371	ASN	CB-CG	-5.64	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1381	TYR	CG-CD1	5.63	1.46	1.39
1	B	1458	GLY	N-CA	5.56	1.54	1.46
1	B	1105	LEU	CG-CD2	5.54	1.72	1.51
1	B	1272	LYS	CB-CG	-5.53	1.37	1.52
1	A	1412	TYR	CD2-CE2	5.43	1.47	1.39
1	A	1114	TYR	CE2-CZ	5.43	1.45	1.38
1	B	1229	GLU	CD-OE1	5.36	1.31	1.25
1	A	1372	GLU	CB-CG	-5.33	1.42	1.52
1	A	1114	TYR	CE1-CZ	5.33	1.45	1.38
1	B	1320	CYS	CB-SG	-5.31	1.73	1.81
1	B	1236	LYS	CG-CD	-5.25	1.34	1.52
1	A	1330	GLU	CG-CD	5.24	1.59	1.51
1	A	1396	LYS	CB-CG	-5.18	1.38	1.52
1	B	1113	CYS	CB-SG	-5.17	1.73	1.81
1	B	1218	LEU	CG-CD2	-5.17	1.32	1.51
1	A	1275	LYS	CB-CG	-5.06	1.38	1.52
1	A	1114	TYR	CG-CD2	5.02	1.45	1.39
1	A	1189	TRP	CB-CG	5.02	1.59	1.50
1	B	1459	LEU	N-CA	5.01	1.56	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1128	VAL	N-CA-C	-9.04	86.58	111.00
1	A	1131	VAL	CB-CA-C	-8.84	94.61	111.40
1	B	1442	HIS	CB-CA-C	-8.38	93.65	110.40
1	B	1218	LEU	CB-CG-CD2	-7.40	98.41	111.00
1	A	1330	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	B	1179	LYS	CB-CA-C	7.17	124.74	110.40
1	B	1175	MET	N-CA-CB	-7.01	97.98	110.60
1	A	1128	VAL	CB-CA-C	-6.63	98.80	111.40
1	A	1255	ILE	CG1-CB-CG2	-6.32	97.50	111.40
1	A	1370	LEU	CA-CB-CG	6.04	129.20	115.30
1	B	1370	LEU	CB-CG-CD1	-5.94	100.91	111.00
1	B	1253	ILE	CG1-CB-CG2	-5.90	98.42	111.40
1	A	1179	LYS	CB-CA-C	-5.41	99.58	110.40
1	B	1336	GLU	CA-CB-CG	5.41	125.29	113.40
1	B	1161	LYS	CA-CB-CG	5.22	124.89	113.40
1	B	1311	MET	CG-SD-CE	-5.20	91.89	100.20
1	B	1377	PHE	CB-CA-C	-5.16	100.09	110.40
1	A	1433	SER	CB-CA-C	-5.14	100.33	110.10
1	B	1353	LEU	CB-CG-CD2	-5.12	102.30	111.00



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1440	LYS	Peptide

## 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	2651	0	2737	90	0
1	B	2802	0	2901	132	0
2	A	80	0	0	4	0
2	B	90	0	0	6	0
All	All	5623	0	5638	219	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 21.

All (219) 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:1346:ILE:HD11	1:B:1349:VAL:CG1	1.57	1.34
1:A:1354:ILE:HG13	2:A:177:HOH:O	1.39	1.20
1:B:1369:ASN:ND2	1:B:1372:GLU:H	1.39	1.19
1:A:1131:VAL:HG22	1:A:1132:ASN:N	1.54	1.18
1:A:1128:VAL:HG12	1:A:1129:THR:N	1.51	1.17
1:A:1346:ILE:HD11	1:A:1349:VAL:HG12	1.28	1.12
1:A:1128:VAL:CG1	1:A:1129:THR:H	1.59	1.09
1:A:1152:ARG:HH11	1:A:1152:ARG:HG2	1.14	1.05
1:B:1346:ILE:CD1	1:B:1349:VAL:HG12	1.86	1.05
1:A:1126:VAL:HG12	1:A:1126:VAL:O	1.57	1.03
1:B:1399:ASN:HB3	2:B:141:HOH:O	1.55	1.03
1:A:1131:VAL:HG22	1:A:1132:ASN:H	0.91	1.03
1:A:1131:VAL:CG2	1:A:1132:ASN:H	1.71	1.00
1:B:1346:ILE:CD1	1:B:1349:VAL:CG1	2.38	1.00
1:A:1122:TYR:O	1:A:1126:VAL:HG23	1.66	0.96
1:A:1176:SER:HB2	2:A:185:HOH:O	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1127:ASN:HD22	1:B:1127:ASN:H	1.02	0.95
1:A:1202:ASN:O	1:A:1205:THR:HG22	1.67	0.94
1:B:1465:ILE:O	1:B:1468:LEU:HD23	1.70	0.92
1:B:1369:ASN:HD22	1:B:1372:GLU:H	1.12	0.91
1:B:1136:VAL:HG12	1:B:1137:LEU:HD13	1.51	0.90
1:A:1111:LEU:O	1:A:1115:THR:HG23	1.72	0.90
1:A:1152:ARG:NH1	1:A:1152:ARG:HG2	1.82	0.89
1:A:1346:ILE:CD1	1:A:1349:VAL:HG12	2.02	0.89
1:B:1127:ASN:H	1:B:1127:ASN:ND2	1.65	0.89
1:B:1129:THR:N	1:B:1130:GLU:HA	1.88	0.89
1:B:1346:ILE:HD11	1:B:1349:VAL:HG12	0.90	0.88
1:B:1369:ASN:ND2	1:B:1372:GLU:N	2.22	0.87
1:A:1132:ASN:OD1	1:A:1132:ASN:N	2.08	0.85
1:B:1367:ILE:HD11	1:B:1373:PHE:HD1	1.42	0.84
1:B:1128:VAL:HG22	1:B:1128:VAL:O	1.78	0.82
1:A:1128:VAL:HG12	1:A:1129:THR:H	0.70	0.81
1:B:1136:VAL:CG1	1:B:1137:LEU:HD13	2.10	0.80
1:B:1462:VAL:O	1:B:1466:ILE:HG13	1.81	0.80
1:B:1127:ASN:N	1:B:1127:ASN:HD22	1.79	0.79
1:A:1126:VAL:CG1	1:A:1126:VAL:O	2.29	0.78
1:A:1205:THR:HG23	1:A:1206:LEU:HD23	1.63	0.78
1:B:1197:PRO:HG3	1:B:1230:THR:HG22	1.66	0.78
1:A:1374:LYS:HE3	2:A:146:HOH:O	1.85	0.77
1:B:1136:VAL:HG12	1:B:1137:LEU:N	2.00	0.76
1:B:1369:ASN:HD21	1:B:1372:GLU:H	1.31	0.76
1:B:1365:LEU:HD11	1:B:1380:TRP:CH2	2.21	0.76
1:B:1330:GLU:OE1	1:B:1333:ARG:NH1	2.19	0.75
1:B:1140:ILE:O	1:B:1144:THR:HB	1.87	0.75
1:A:1205:THR:HG23	1:A:1206:LEU:CD2	2.16	0.75
1:B:1440:LYS:HA	1:B:1441:ASN:O	1.86	0.74
1:A:1176:SER:CB	2:A:185:HOH:O	2.30	0.74
1:A:1406:PRO:HG2	1:A:1409:ILE:HD12	1.69	0.74
1:A:1253:ILE:HD11	1:A:1279:PHE:CG	2.23	0.74
1:A:1202:ASN:O	1:A:1205:THR:CG2	2.38	0.72
1:B:1238:TYR:HE1	1:B:1300:ILE:HD12	1.55	0.72
1:A:1140:ILE:O	1:A:1144:THR:HB	1.90	0.72
1:B:1253:ILE:HG13	1:B:1255:ILE:CD1	2.20	0.72
1:B:1320:CYS:O	1:B:1394:LYS:NZ	2.19	0.71
1:B:1377:PHE:CD1	1:B:1377:PHE:C	2.66	0.69
1:B:1266:LYS:HB2	2:B:74:HOH:O	1.92	0.69
1:A:1296:MET:HE3	1:A:1443:LEU:HD21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:ARG:CG	1:A:1152:ARG:NH1	2.49	0.68
1:A:1226:LEU:O	1:A:1230:THR:HB	1.94	0.68
1:B:1420:GLU:HG3	1:B:1428:MET:CE	2.24	0.67
1:B:1129:THR:N	1:B:1130:GLU:CA	2.56	0.67
1:B:1296:MET:CE	1:B:1442:HIS:O	2.43	0.66
1:A:1350:ARG:HB2	2:B:83:HOH:O	1.96	0.66
1:A:1377:PHE:CE1	1:B:1379:PHE:HZ	2.14	0.66
1:B:1253:ILE:HG13	1:B:1255:ILE:HD11	1.77	0.65
1:B:1305:LEU:CD1	1:B:1349:VAL:HB	2.25	0.65
1:B:1369:ASN:HD21	1:B:1372:GLU:N	1.92	0.65
1:A:1128:VAL:CG1	1:A:1129:THR:N	2.29	0.64
1:B:1365:LEU:HD11	1:B:1380:TRP:CZ2	2.32	0.64
1:B:1226:LEU:O	1:B:1230:THR:HB	1.98	0.64
1:B:1238:TYR:HE1	1:B:1300:ILE:CD1	2.11	0.63
1:A:1186:GLY:HA3	1:A:1241:TRP:NE1	2.13	0.63
1:B:1196:LEU:HB3	1:B:1230:THR:HG21	1.80	0.62
1:A:1115:THR:O	1:A:1119:THR:HG22	1.99	0.62
1:B:1440:LYS:CA	1:B:1441:ASN:O	2.47	0.62
1:B:1346:ILE:HA	2:B:20:HOH:O	2.00	0.62
1:B:1293:VAL:HG11	1:B:1444:ARG:HB3	1.82	0.61
1:B:1369:ASN:O	1:B:1369:ASN:ND2	2.33	0.61
1:A:1197:PRO:HG3	1:A:1230:THR:HG22	1.83	0.61
1:A:1296:MET:HE3	1:A:1443:LEU:CD2	2.30	0.61
1:B:1465:ILE:O	1:B:1468:LEU:CD2	2.47	0.61
1:A:1369:ASN:OD1	1:A:1372:GLU:HG3	2.00	0.60
1:B:1365:LEU:CD1	1:B:1380:TRP:CZ2	2.84	0.60
1:B:1238:TYR:CE1	1:B:1300:ILE:HD12	2.37	0.60
1:A:1317:ILE:O	1:A:1394:LYS:NZ	2.34	0.60
1:B:1317:ILE:O	1:B:1394:LYS:HE3	2.02	0.59
1:B:1440:LYS:HA	1:B:1441:ASN:C	2.18	0.59
1:B:1129:THR:H	1:B:1130:GLU:HA	1.67	0.59
1:B:1459:LEU:O	1:B:1463:SER:CB	2.51	0.59
1:B:1178:PRO:HG2	1:B:1181:GLU:HB2	1.86	0.58
1:B:1306:LYS:HE2	1:B:1352:ASN:OD1	2.03	0.58
1:B:1317:ILE:O	1:B:1394:LYS:CE	2.52	0.58
1:A:1206:LEU:N	1:A:1206:LEU:HD23	2.19	0.57
1:A:1245:PHE:CE2	1:A:1246:MET:HE2	2.39	0.57
1:B:1111:LEU:O	1:B:1115:THR:HG23	2.05	0.57
1:B:1296:MET:HE3	1:B:1443:LEU:HD21	1.85	0.57
1:B:1377:PHE:CD1	1:B:1377:PHE:O	2.57	0.57
1:B:1439:ALA:C	1:B:1441:ASN:O	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1302:ASN:HD22	1:B:1352:ASN:ND2	2.04	0.55
1:B:1296:MET:HE3	1:B:1439:ALA:HB1	1.89	0.55
1:B:1296:MET:CE	1:B:1439:ALA:HB1	2.36	0.55
1:B:1419:ARG:NH1	2:B:67:HOH:O	2.33	0.55
1:B:1376:LEU:O	1:B:1379:PHE:HB2	2.07	0.55
1:B:1302:ASN:HD22	1:B:1352:ASN:HD21	1.55	0.54
1:B:1140:ILE:HG22	1:B:1192:ASN:OD1	2.06	0.54
1:B:1296:MET:HE3	1:B:1443:LEU:CD2	2.38	0.54
1:B:1381:TYR:HA	2:B:172:HOH:O	2.06	0.54
1:B:1128:VAL:CG2	1:B:1128:VAL:O	2.49	0.54
1:B:1305:LEU:HD13	1:B:1349:VAL:HB	1.90	0.53
1:B:1398:ALA:HA	1:B:1399:ASN:OD1	2.08	0.53
1:A:1195:ARG:NH2	1:A:1291:GLN:O	2.41	0.53
1:A:1119:THR:HG23	1:A:1120:GLU:HG2	1.91	0.53
1:B:1369:ASN:HD21	1:B:1371:ASN:CA	2.20	0.53
1:B:1187:ILE:HD11	1:B:1283:PHE:HE2	1.73	0.53
1:B:1305:LEU:HD21	1:B:1342:PHE:CE1	2.43	0.53
1:A:1305:LEU:HD21	1:A:1342:PHE:CE1	2.44	0.53
1:A:1342:PHE:CB	1:A:1349:VAL:HG11	2.39	0.53
1:B:1459:LEU:O	1:B:1463:SER:OG	2.21	0.52
1:B:1249:ALA:O	1:B:1253:ILE:HG12	2.09	0.52
1:A:1178:PRO:HG2	1:A:1181:GLU:HB2	1.91	0.52
1:A:1347:GLU:HG2	1:A:1348:ASP:H	1.73	0.52
1:B:1136:VAL:HG12	1:B:1137:LEU:CD1	2.31	0.52
1:B:1190:LEU:O	1:B:1194:SER:HB3	2.10	0.52
1:B:1136:VAL:CG1	1:B:1137:LEU:CD1	2.86	0.52
1:B:1365:LEU:HD11	1:B:1380:TRP:HH2	1.71	0.52
1:B:1367:ILE:HD11	1:B:1373:PHE:CD1	2.32	0.52
1:B:1365:LEU:CD1	1:B:1380:TRP:HZ2	2.22	0.51
1:A:1123:LEU:HD21	1:A:1139:PRO:HB3	1.91	0.51
1:B:1369:ASN:ND2	1:B:1371:ASN:N	2.58	0.51
1:A:1127:ASN:C	1:A:1128:VAL:O	2.43	0.51
1:B:1369:ASN:C	1:B:1369:ASN:ND2	2.63	0.51
1:B:1354:ILE:HG13	1:B:1382:ALA:HB2	1.93	0.51
1:A:1296:MET:CE	1:A:1443:LEU:CD2	2.89	0.50
1:B:1187:ILE:HD11	1:B:1283:PHE:CE2	2.47	0.50
1:B:1253:ILE:CG1	1:B:1255:ILE:HD11	2.41	0.50
1:A:1281:ASN:ND2	1:A:1341:TRP:HE1	2.10	0.50
1:A:1202:ASN:C	1:A:1205:THR:HG22	2.32	0.49
1:A:1253:ILE:HD11	1:A:1279:PHE:CD2	2.46	0.49
1:A:1128:VAL:O	1:A:1129:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1183:MET:HE1	1:B:1283:PHE:HA	1.95	0.49
1:B:1439:ALA:O	1:B:1443:LEU:HG	2.11	0.49
1:B:1367:ILE:CD1	1:B:1373:PHE:HD1	2.21	0.49
1:B:1369:ASN:HD22	1:B:1372:GLU:N	1.96	0.49
1:A:1115:THR:HG22	1:A:1162:PHE:HD1	1.78	0.49
1:A:1420:GLU:OE2	1:A:1424:LEU:HD12	2.13	0.48
1:B:1376:LEU:O	1:B:1379:PHE:N	2.40	0.48
1:B:1302:ASN:ND2	1:B:1352:ASN:HD21	2.12	0.48
1:A:1339:VAL:HG13	1:A:1349:VAL:HG21	1.96	0.48
1:A:1187:ILE:HD11	1:A:1283:PHE:HE1	1.80	0.47
1:B:1365:LEU:C	1:B:1366:LYS:HG2	2.35	0.47
1:B:1459:LEU:O	1:B:1463:SER:HB2	2.14	0.47
1:B:1238:TYR:CE1	1:B:1300:ILE:CD1	2.96	0.47
1:A:1342:PHE:HB3	1:A:1349:VAL:HG11	1.96	0.47
1:A:1169:THR:O	1:A:1173:ILE:HG13	2.14	0.47
1:B:1127:ASN:N	1:B:1127:ASN:ND2	2.41	0.47
1:A:1205:THR:HG23	1:A:1206:LEU:HD21	1.95	0.47
1:B:1183:MET:CE	1:B:1283:PHE:HA	2.45	0.46
1:A:1236:LYS:O	1:A:1240:THR:HG23	2.14	0.46
1:B:1369:ASN:HD21	1:B:1371:ASN:HB2	1.80	0.46
1:A:1268:SER:HB2	1:A:1270:ASP:CG	2.36	0.46
1:B:1384:ASN:HB2	1:B:1385:PRO:CD	2.45	0.46
1:A:1255:ILE:HA	1:A:1258:MET:HE3	1.96	0.46
1:A:1123:LEU:HD22	1:A:1189:TRP:CZ3	2.51	0.45
1:A:1326:LYS:HD2	1:A:1326:LYS:HA	1.75	0.45
1:B:1323:LEU:HD13	1:B:1363:LEU:HD11	1.98	0.45
1:A:1123:LEU:CD2	1:A:1139:PRO:HB3	2.46	0.45
1:A:1175:MET:HB3	1:A:1175:MET:HE3	1.75	0.45
1:B:1296:MET:HE2	1:B:1442:HIS:O	2.16	0.45
1:B:1343:GLU:N	1:B:1344:PRO:HD2	2.31	0.45
1:B:1101:ASN:O	1:B:1104:LEU:HB3	2.17	0.44
1:B:1144:THR:HG23	1:B:1199:PHE:CE1	2.52	0.44
1:A:1342:PHE:HB2	1:A:1349:VAL:HG11	2.00	0.44
1:A:1370:LEU:HD12	1:A:1371:ASN:N	2.32	0.44
1:A:1131:VAL:CG2	1:A:1132:ASN:N	2.31	0.44
1:B:1169:THR:O	1:B:1173:ILE:HG13	2.17	0.44
1:B:1183:MET:HE2	1:B:1286:VAL:HG21	2.00	0.44
1:B:1441:ASN:O	1:B:1442:HIS:CB	2.65	0.44
1:A:1128:VAL:C	1:A:1129:THR:HG23	2.37	0.44
1:B:1440:LYS:N	1:B:1441:ASN:O	2.51	0.44
1:A:1119:THR:OG1	1:A:1169:THR:OG1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1420:GLU:HG3	1:B:1428:MET:HE1	2.00	0.44
1:B:1441:ASN:O	1:B:1442:HIS:HB2	2.17	0.44
1:A:1236:LYS:O	1:A:1240:THR:CG2	2.66	0.44
1:B:1196:LEU:HB3	1:B:1230:THR:CG2	2.46	0.43
1:B:1277:PHE:CE1	1:B:1341:TRP:HB2	2.53	0.43
1:B:1322:ALA:O	1:B:1323:LEU:HD23	2.18	0.43
1:B:1253:ILE:CD1	1:B:1255:ILE:HD11	2.48	0.43
1:A:1253:ILE:O	1:A:1254:GLU:HB2	2.19	0.43
1:B:1326:LYS:HA	1:B:1326:LYS:HD2	1.78	0.43
1:B:1299:LYS:NZ	1:B:1303:ASP:OD2	2.52	0.43
1:B:1327:TYR:CE2	1:B:1331:VAL:HG21	2.54	0.43
1:B:1373:PHE:CE2	1:B:1377:PHE:HD2	2.37	0.43
1:A:1296:MET:HE2	1:A:1443:LEU:HD23	2.00	0.42
1:A:1110:ASP:O	1:A:1111:LEU:C	2.56	0.42
1:A:1335:ILE:HG21	1:A:1357:ILE:HD11	2.01	0.42
1:B:1281:ASN:ND2	1:B:1341:TRP:HE1	2.17	0.42
1:B:1467:LYS:O	1:B:1468:LEU:HB2	2.19	0.42
1:A:1379:PHE:CD1	1:B:1350:ARG:CD	3.02	0.42
1:A:1115:THR:CG2	1:A:1162:PHE:HD1	2.32	0.42
1:A:1327:TYR:CE2	1:A:1331:VAL:HG21	2.54	0.42
1:B:1216:ASP:O	1:B:1220:LEU:HG	2.19	0.42
1:B:1305:LEU:HD21	1:B:1342:PHE:CZ	2.54	0.42
1:B:1396:LYS:HA	1:B:1397:PRO:HD3	1.95	0.42
1:A:1331:VAL:HG11	1:A:1360:VAL:HG11	2.01	0.42
1:B:1354:ILE:HG13	1:B:1382:ALA:CB	2.50	0.42
1:A:1296:MET:HE3	1:A:1439:ALA:HB1	2.01	0.41
1:B:1309:ASN:HB2	1:B:1353:LEU:HD23	2.01	0.41
1:A:1114:TYR:CE2	1:A:1115:THR:HG22	2.56	0.41
1:A:1338:LEU:HD23	1:A:1338:LEU:C	2.41	0.41
1:A:1163:ILE:HD13	1:A:1163:ILE:HA	1.99	0.41
1:A:1253:ILE:HG22	1:A:1253:ILE:O	2.19	0.41
1:B:1128:VAL:C	1:B:1130:GLU:CB	2.89	0.41
1:A:1327:TYR:O	1:A:1331:VAL:HG23	2.21	0.41
1:B:1358:GLN:CD	1:B:1382:ALA:HB3	2.41	0.41
1:B:1415:ASN:ND2	1:B:1418:LYS:NZ	2.69	0.41
1:A:1378:ASP:O	1:B:1361:LYS:NZ	2.47	0.40
1:A:1296:MET:HE1	1:A:1442:HIS:HB2	2.02	0.40
1:B:1338:LEU:HD23	1:B:1338:LEU:C	2.42	0.40
1:A:1320:CYS:O	1:A:1394:LYS:CE	2.70	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	318/386 (82%)	301 (95%)	14 (4%)	3 (1%)	20	23
1	B	338/386 (88%)	317 (94%)	18 (5%)	3 (1%)	20	23
All	All	656/772 (85%)	618 (94%)	32 (5%)	6 (1%)	20	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1179	LYS
1	B	1133	GLY
1	B	1131	VAL
1	B	1377	PHE
1	A	1128	VAL
1	A	1131	VAL

### 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	300/349 (86%)	268 (89%)	32 (11%)	8	8
1	B	317/349 (91%)	278 (88%)	39 (12%)	5	6
All	All	617/698 (88%)	546 (88%)	71 (12%)	6	7

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1109	MET
1	A	1112	ASN
1	A	1115	THR
1	A	1116	LEU
1	A	1125	LYS
1	A	1132	ASN
1	A	1144	THR
1	A	1152	ARG
1	A	1160	SER
1	A	1165	LYS
1	A	1168	LEU
1	A	1179	LYS
1	A	1180	ASP
1	A	1181	GLU
1	A	1204	LYS
1	A	1205	THR
1	A	1206	LEU
1	A	1218	LEU
1	A	1230	THR
1	A	1240	THR
1	A	1247	LYS
1	A	1255	ILE
1	A	1266	LYS
1	A	1275	LYS
1	A	1287	LEU
1	A	1294	ASP
1	A	1332	ASP
1	A	1339	VAL
1	A	1346	ILE
1	A	1370	LEU
1	A	1379	PHE
1	A	1396	LYS
1	B	1105	LEU
1	B	1107	LEU
1	B	1111	LEU
1	B	1115	THR
1	B	1116	LEU
1	B	1127	ASN
1	B	1131	VAL
1	B	1135	ASN
1	B	1136	VAL
1	B	1144	THR
1	B	1157	ILE

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Mol	Chain	Res	Type
1	B	1160	SER
1	B	1168	LEU
1	B	1175	MET
1	B	1179	LYS
1	B	1204	LYS
1	B	1215	LYS
1	B	1218	LEU
1	B	1230	THR
1	B	1236	LYS
1	B	1243	VAL
1	B	1253	ILE
1	B	1266	LYS
1	B	1298	THR
1	B	1311	MET
1	B	1317	ILE
1	B	1326	LYS
1	B	1339	VAL
1	B	1343	GLU
1	B	1346	ILE
1	B	1366	LYS
1	B	1367	ILE
1	B	1369	ASN
1	B	1374	LYS
1	B	1375	LEU
1	B	1379	PHE
1	B	1392	LEU
1	B	1405	VAL
1	B	1411	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1112	ASN
1	A	1202	ASN
1	A	1267	ASN
1	A	1281	ASN
1	A	1334	ASN
1	A	1407	ASN
1	A	1415	ASN
1	B	1127	ASN
1	B	1281	ASN
1	B	1302	ASN

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Mol	Chain	Res	Type
1	B	1369	ASN
1	B	1415	ASN
1	B	1442	HIS

### 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<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	326/386 (84%)	0.36	33 (10%) <b>8</b> <b>11</b>	11, 34, 66, 105	33 (10%)
1	B	346/386 (89%)	0.35	32 (9%) <b>10</b> <b>13</b>	11, 36, 60, 83	56 (16%)
All	All	672/772 (87%)	0.36	65 (9%) <b>8</b> <b>12</b>	11, 35, 64, 105	89 (13%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1178	PRO	6.2
1	A	1128	VAL	5.7
1	A	1265	PHE	5.2
1	B	1128	VAL	5.1
1	B	1445	TYR	4.9
1	A	1175	MET	4.9
1	B	1459	LEU	4.4
1	B	1129	THR	4.3
1	B	1403	ALA	4.3
1	B	1398	ALA	4.2
1	A	1176	SER	4.2
1	A	1129	THR	4.0
1	A	1119	THR	3.7
1	A	1267	ASN	3.7
1	A	1205	THR	3.7
1	B	1346	ILE	3.3
1	A	1118	VAL	3.3
1	B	1345	ARG	3.2
1	B	1207	TYR	3.1
1	A	1131	VAL	3.1
1	B	1134	ASP	3.0
1	B	1444	ARG	3.0
1	B	1294	ASP	2.9
1	A	1172	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	1172	SER	2.9
1	A	1397	PRO	2.8
1	B	1182	THR	2.8
1	B	1404	GLY	2.7
1	B	1467	LYS	2.7
1	B	1397	PRO	2.7
1	B	1215	LYS	2.7
1	A	1376	LEU	2.6
1	A	1180	ASP	2.6
1	B	1468	LEU	2.6
1	A	1107	LEU	2.6
1	A	1347	GLU	2.6
1	B	1441	ASN	2.5
1	B	1102	PRO	2.5
1	A	1196	LEU	2.5
1	B	1178	PRO	2.5
1	B	1399	ASN	2.5
1	A	1398	ALA	2.4
1	B	1356	ILE	2.4
1	B	1113	CYS	2.4
1	A	1105	LEU	2.4
1	B	1130	GLU	2.4
1	A	1103	ASP	2.4
1	A	1152	ARG	2.4
1	A	1370	LEU	2.4
1	A	1113	CYS	2.3
1	A	1106	GLU	2.3
1	B	1460	ALA	2.3
1	B	1293	VAL	2.2
1	B	1312	LEU	2.2
1	A	1122	TYR	2.2
1	A	1270	ASP	2.1
1	A	1230	THR	2.1
1	A	1346	ILE	2.1
1	A	1266	LYS	2.1
1	B	1379	PHE	2.1
1	B	1362	ILE	2.1
1	A	1112	ASN	2.1
1	B	1190	LEU	2.1
1	A	1104	LEU	2.0
1	A	1216	ASP	2.0

## 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.