



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:02 AM UTC

PDB ID : 3MMI / pdb_00003mmi
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

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

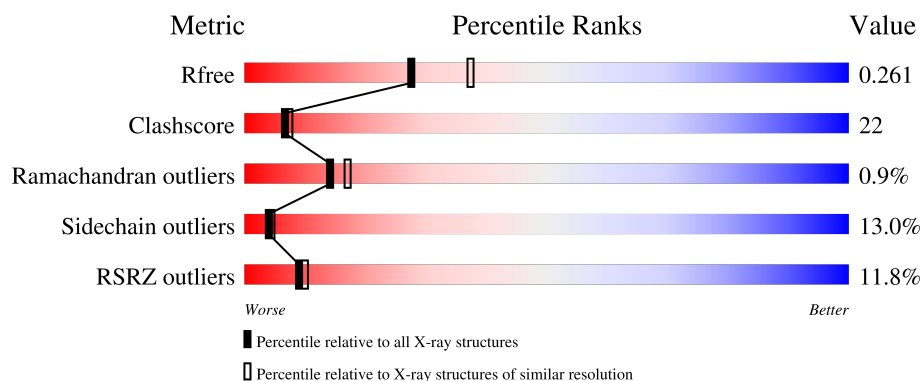
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	386	10% 50% 26% 6% • 16%
1	B	386	11% 50% 28% 11% • 10%

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

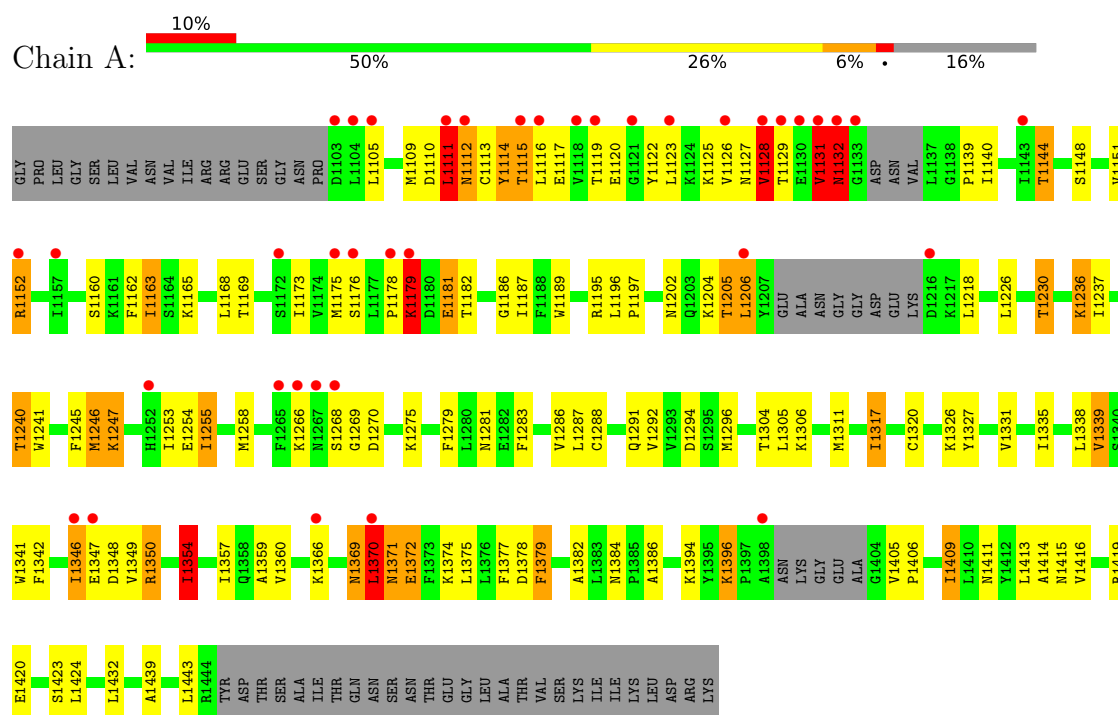
- Molecule 2 is water.

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

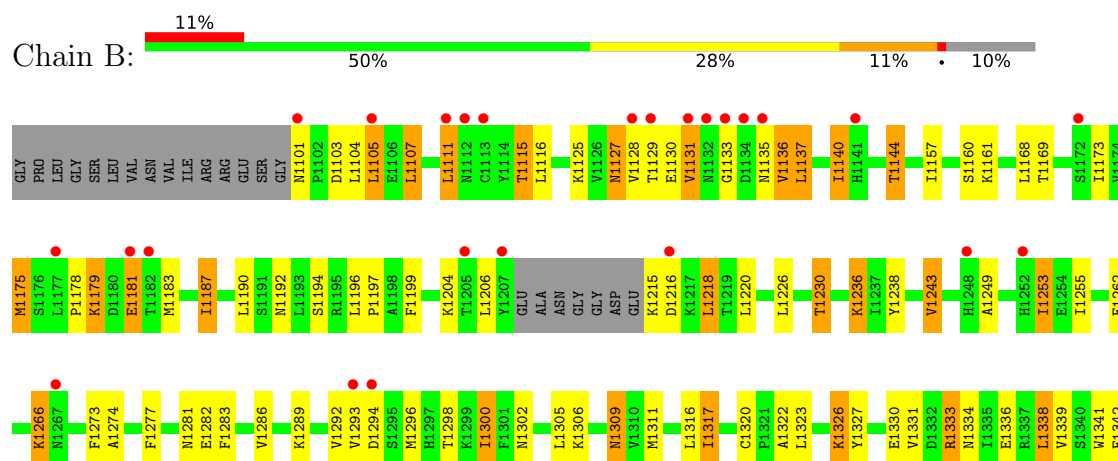
3 Residue-property plots

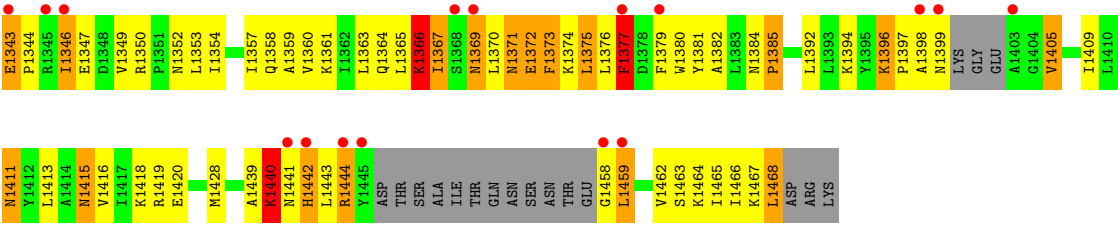
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Myosin-4



• Molecule 1: Myosin-4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.48Å 120.99Å 157.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.51 – 2.30 30.51 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.51-2.30) 98.0 (30.51-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5623	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	1.63	19/2702 (0.7%)	1.47	31/3654 (0.8%)
1	B	1.69	39/2855 (1.4%)	1.40	24/3862 (0.6%)
All	All	1.66	58/5557 (1.0%)	1.44	55/7516 (0.7%)

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 (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1125	LYS	CA-CB	-13.79	1.34	1.54
1	A	1416	VAL	CA-CB	12.01	1.68	1.54
1	B	1416	VAL	CA-CB	11.37	1.67	1.54
1	A	1382	ALA	CA-C	9.13	1.65	1.52
1	B	1459	LEU	N-CA	8.60	1.56	1.46
1	B	1336	GLU	CB-CG	-7.81	1.29	1.52
1	A	1247	LYS	CG-CD	7.25	1.74	1.52
1	B	1334	ASN	CA-C	-6.92	1.43	1.52
1	A	1117	GLU	CB-CG	-6.65	1.32	1.52
1	B	1409	ILE	CA-CB	6.58	1.63	1.54
1	A	1317	ILE	C-O	-6.53	1.16	1.24
1	B	1333	ARG	N-CA	6.34	1.54	1.46
1	A	1111	LEU	CA-CB	6.11	1.63	1.53
1	A	1369	ASN	CA-C	-6.02	1.45	1.52
1	B	1468	LEU	C-O	6.01	1.35	1.23
1	B	1218	LEU	CG-CD2	-6.00	1.32	1.52
1	A	1413	LEU	N-CA	6.00	1.53	1.46
1	B	1370	LEU	CB-CG	-6.00	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1105	LEU	CG-CD2	5.99	1.72	1.52
1	B	1243	VAL	CA-CB	5.95	1.62	1.54
1	B	1236	LYS	CG-CD	-5.95	1.34	1.52
1	B	1309	ASN	CA-C	5.92	1.60	1.52
1	A	1350	ARG	CG-CD	-5.87	1.34	1.52
1	A	1414	ALA	N-CA	5.87	1.53	1.46
1	B	1107	LEU	CA-C	5.83	1.60	1.52
1	B	1206	LEU	CA-CB	-5.75	1.43	1.53
1	B	1289	LYS	CE-NZ	-5.67	1.32	1.49
1	A	1432	LEU	N-CA	5.63	1.52	1.45
1	B	1364	GLN	C-O	-5.61	1.16	1.24
1	B	1371	ASN	CB-CG	-5.59	1.38	1.52
1	B	1385	PRO	CA-C	5.56	1.60	1.52
1	B	1366	LYS	CG-CD	5.55	1.69	1.52
1	A	1359	ALA	N-CA	5.54	1.53	1.46
1	B	1458	GLY	N-CA	5.52	1.54	1.45
1	A	1384	ASN	CA-CB	5.52	1.59	1.53
1	B	1409	ILE	CG1-CD1	-5.50	1.30	1.51
1	B	1464	LYS	C-O	5.49	1.30	1.24
1	B	1292	VAL	CA-CB	5.44	1.60	1.54
1	B	1357	ILE	C-O	-5.38	1.18	1.24
1	B	1459	LEU	C-O	5.37	1.30	1.24
1	B	1300	ILE	CG1-CD1	-5.33	1.30	1.51
1	A	1288	CYS	N-CA	5.32	1.52	1.46
1	A	1286	VAL	CA-CB	-5.31	1.48	1.54
1	B	1262	GLU	CG-CD	5.30	1.65	1.52
1	B	1140	ILE	CA-CB	5.29	1.61	1.54
1	B	1274	ALA	CA-CB	5.28	1.61	1.53
1	B	1372	GLU	C-O	-5.28	1.18	1.24
1	B	1413	LEU	N-CA	5.27	1.52	1.46
1	A	1196	LEU	N-CA	5.26	1.51	1.46
1	B	1440	LYS	CA-C	-5.23	1.47	1.53
1	A	1419	ARG	C-O	-5.17	1.18	1.24
1	B	1187	ILE	CA-CB	5.17	1.60	1.54
1	B	1338	LEU	N-CA	5.13	1.52	1.46
1	B	1373	PHE	C-O	-5.12	1.18	1.24
1	B	1359	ALA	C-O	-5.10	1.18	1.24
1	B	1375	LEU	C-O	-5.08	1.18	1.24
1	A	1151	VAL	CA-CB	5.03	1.61	1.54
1	A	1237	ILE	C-O	-5.02	1.18	1.24

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1128	VAL	N-CA-C	-10.94	86.58	109.34
1	A	1132	ASN	N-CA-C	10.74	124.38	110.53
1	A	1131	VAL	CB-CA-C	-10.17	94.61	111.29
1	B	1179	LYS	CB-CA-C	8.44	124.74	110.74
1	B	1442	HIS	CB-CA-C	-8.43	93.65	110.42
1	B	1175	MET	N-CA-CB	-8.26	97.98	110.12
1	A	1371	ASN	N-CA-C	8.01	120.00	111.28
1	B	1415	ASN	N-CA-C	7.94	119.93	111.28
1	A	1128	VAL	CB-CA-C	-7.62	98.80	111.29
1	B	1103	ASP	N-CA-C	-7.18	103.49	111.82
1	B	1347	GLU	N-CA-C	7.11	119.70	111.02
1	B	1273	PHE	N-CA-C	6.89	119.64	111.71
1	A	1386	ALA	N-CA-C	-6.82	103.93	111.36
1	A	1354	ILE	N-CA-C	6.77	117.53	110.62
1	B	1409	ILE	N-CA-C	-6.40	104.03	111.00
1	A	1409	ILE	N-CA-C	6.38	117.16	110.72
1	A	1246	MET	N-CA-C	6.36	119.20	111.82
1	A	1113	CYS	N-CA-C	-6.33	104.00	111.03
1	A	1423	SER	N-CA-C	6.22	119.34	111.69
1	B	1411	ASN	CB-CA-C	-6.15	101.23	110.88
1	A	1415	ASN	N-CA-C	6.13	117.96	111.28
1	B	1444	ARG	N-CA-C	6.03	118.24	109.07
1	A	1370	LEU	N-CA-C	-5.96	105.27	112.54
1	A	1269	GLY	CA-C-N	5.93	128.71	120.29
1	A	1269	GLY	C-N-CA	5.93	128.71	120.29
1	A	1114	TYR	N-CA-C	5.91	118.67	111.82
1	A	1148	SER	N-CA-C	5.88	118.47	111.71
1	A	1411	ASN	N-CA-C	5.75	117.23	110.97
1	B	1218	LEU	CD1-CG-CD2	5.69	123.33	110.80
1	A	1359	ALA	N-CA-C	-5.68	105.00	111.14
1	A	1396	LYS	CA-CB-CG	-5.67	102.76	114.10
1	B	1316	LEU	N-CA-C	-5.66	105.11	111.28
1	B	1357	ILE	N-CA-C	5.63	116.28	110.36
1	A	1317	ILE	CB-CA-C	-5.61	104.48	112.22
1	B	1336	GLU	CA-CB-CG	5.59	125.29	114.10
1	B	1181	GLU	CA-CB-CG	-5.53	103.05	114.10
1	A	1179	LYS	CB-CA-C	-5.45	99.58	110.42
1	B	1366	LYS	CA-C-N	-5.43	113.18	120.95
1	B	1366	LYS	C-N-CA	-5.43	113.18	120.95
1	B	1161	LYS	CA-CB-CG	5.39	124.89	114.10
1	A	1182	THR	N-CA-C	5.31	117.07	111.28
1	B	1405	VAL	CB-CA-C	5.31	116.20	111.00
1	B	1181	GLU	CB-CG-CD	-5.29	103.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1405	VAL	N-CA-C	5.21	113.87	109.02
1	B	1377	PHE	CB-CA-C	-5.19	100.09	110.42
1	A	1306	LYS	N-CA-C	-5.17	105.64	111.28
1	A	1179	LYS	N-CA-C	5.17	121.81	110.80
1	A	1366	LYS	CA-C-N	-5.14	116.45	122.93
1	A	1366	LYS	C-N-CA	-5.14	116.45	122.93
1	A	1405	VAL	N-CA-C	-5.11	103.94	108.95
1	B	1300	ILE	N-CA-C	-5.10	105.41	110.62
1	B	1294	ASP	N-CA-C	5.06	116.48	110.97
1	A	1405	VAL	CB-CA-C	5.03	116.32	110.89
1	A	1269	GLY	N-CA-C	-5.02	108.40	114.92
1	A	1372	GLU	O-C-N	5.01	127.43	122.12

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	135	0
2	A	80	0	0	4	0
2	B	90	0	0	6	0
All	All	5623	0	5638	222	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 22.

All (222) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1131:VAL:HG22	1:A:1132:ASN:N	1.54	1.09
1:A:1152:ARG:HG2	1:A:1152:ARG:HH11	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:1128:VAL:HG12	1:A:1129:THR:N	1.51	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
1:B:1127:ASN:HD22	1:B:1127:ASN:H	1.02	0.95
1:A:1296:MET:HE3	1:A:1443:LEU:CD2	1.97	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:1296:MET:HE3	1:A:1443:LEU:HD21	1.52	0.90
1:A:1111:LEU:O	1:A:1115:THR:HG23	1.72	0.90
1:A:1152:ARG:HG2	1:A:1152:ARG:NH1	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:1296:MET:HE1	1:B:1439:ALA:HB1	1.56	0.88
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:N	1:A:1132:ASN:OD1	2.08	0.85
1:B:1367:ILE:HD11	1:B:1373:PHE:HD1	1.42	0.84
1:B:1128:VAL:O	1:B:1128:VAL:HG22	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:HD22	1:B:1127:ASN:N	1.79	0.79
1:B:1296:MET:HE3	1:B:1443:LEU:CD2	2.13	0.79
1:A:1126:VAL:O	1:A:1126:VAL:CG1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1365:LEU:HD11	1:B:1380:TRP:CH2	2.21	0.76
1:B:1369:ASN:HD21	1:B:1372:GLU:H	1.31	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:B:1377:PHE:CD1	1:B:1377:PHE:C	2.66	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:1183:MET:HE3	1:B:1283:PHE:HA	1.74	0.69
1:B:1266:LYS:HB2	2:B:74:HOH:O	1.92	0.69
1:B:1440:LYS:HA	1:B:1441:ASN:C	2.18	0.69
1:B:1296:MET:HE3	1:B:1443:LEU:HD21	1.75	0.68
1:A:1152:ARG:NH1	1:A:1152:ARG:CG	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:A:1296:MET:HE3	1:A:1443:LEU:HD23	1.78	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:1296:MET:HE3	1:B:1443:LEU:HD23	1.78	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:A:1255:ILE:HG22	1:A:1311:MET:HE1	1.80	0.64
1:B:1183:MET:HE2	1:B:1286:VAL:HG21	1.78	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:ND2	1:B:1369:ASN:O	2.33	0.61
1:A:1197:PRO:HG3	1:A:1230:THR:HG22	1.83	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:1439:ALA:C	1:B:1441:ASN:O	2.44	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: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:1296:MET:HE1	1:A:1439:ALA:HB1	1.86	0.58
1:A:1206:LEU:HD23	1:A:1206:LEU:N	2.19	0.57
1:B:1111:LEU:O	1:B:1115:THR:HG23	2.05	0.57
1:B:1377:PHE:CD1	1:B:1377:PHE:O	2.57	0.57
1:B:1369:ASN:ND2	1:B:1369:ASN:C	2.63	0.56
1:B:1302:ASN:HD22	1:B:1352:ASN:ND2	2.04	0.55
1:A:1127:ASN:C	1:A:1128:VAL:O	2.43	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:A:1202:ASN:C	1:A:1205:THR:HG22	2.32	0.54
1:B:1381:TYR:HA	2:B:172:HOH:O	2.06	0.54
1:B:1128:VAL:O	1:B:1128:VAL:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1365:LEU:C	1:B:1366:LYS:HG2	2.35	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:1296:MET:HE2	1:B:1442:HIS:O	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:B:1296:MET:CE	1:B:1439:ALA:HB1	2.36	0.51
1:B:1354:ILE:HG13	1:B:1382:ALA:HB2	1.93	0.51
1:A:1268:SER:HB2	1:A:1270:ASP:CG	2.36	0.51
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: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
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:1128:VAL:C	1:A:1129:THR:HG23	2.37	0.48
1:A:1420:GLU:OE2	1:A:1424:LEU:HD12	2.13	0.48
1:A:1246:MET:HE3	1:A:1304:THR:HG23	1.95	0.48
1:B:1376:LEU:O	1:B:1379:PHE:N	2.40	0.48
1:B:1420:GLU:HG3	1:B:1428:MET:HE1	1.95	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:A:1255:ILE:CG2	1:A:1311:MET:HE1	2.42	0.47
1:A:1110:ASP:O	1:A:1111:LEU:C	2.56	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:1169:THR:O	1:A:1173:ILE:HG13	2.14	0.47
1:A:1342:PHE:HB3	1:A:1349:VAL:HG11	1.96	0.47
1:B:1127:ASN:ND2	1:B:1127:ASN:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:THR:HG23	1:A:1206:LEU:HD21	1.95	0.47
1:A:1255:ILE:HA	1:A:1258:MET:HE3	1.95	0.46
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:B:1384:ASN:HB2	1:B:1385:PRO:CD	2.45	0.46
1:A:1338:LEU:C	1:A:1338:LEU:HD23	2.41	0.46
1:B:1128:VAL:C	1:B:1130:GLU:CB	2.89	0.46
1:A:1123:LEU:HD22	1:A:1189:TRP:CZ3	2.51	0.45
1:B:1358:GLN:CD	1:B:1382:ALA:HB3	2.41	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:B:1338:LEU:C	1:B:1338:LEU:HD23	2.42	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:B:1169:THR:O	1:B:1173:ILE:HG13	2.17	0.44
1:B:1441:ASN:O	1:B:1442:HIS:CB	2.65	0.44
1:B:1440:LYS:N	1:B:1441:ASN:O	2.51	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:A:1245:PHE:CE2	1:A:1246:MET:HE2	2.53	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:B:1183:MET:HE1	1:B:1282:GLU:HG2	2.01	0.43
1:A:1253:ILE:O	1:A:1254:GLU:HB2	2.19	0.43
1:B:1326:LYS:HD2	1:B:1326:LYS:HA	1.78	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: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:1110:ASP:C	1:A:1112:ASN:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:VAL:C	1:B:1130:GLU:HB3	2.44	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:B:1309:ASN:HB2	1:B:1353:LEU:HD23	2.01	0.41
1:A:1370:LEU:CD1	1:A:1370:LEU:C	2.93	0.41
1:A:1114:TYR:CE2	1:A:1115:THR:HG22	2.56	0.41
1:B:1327:TYR:CD2	1:B:1327:TYR:C	2.98	0.41
1:A:1163:ILE:HD13	1:A:1163:ILE:HA	1.99	0.41
1:A:1253:ILE:O	1:A:1253:ILE:HG22	2.19	0.41
1:A:1327:TYR:O	1:A:1331:VAL:HG23	2.21	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: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%)	14	17
1	B	338/386 (88%)	317 (94%)	18 (5%)	3 (1%)	14	17
All	All	656/772 (85%)	618 (94%)	32 (5%)	6 (1%)	14	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1179	LYS
1	B	1133	GLY

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Mol	Chain	Res	Type
1	B	1131	VAL
1	B	1377	PHE
1	A	1128	VAL
1	A	1131	VAL

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	300/349 (86%)	262 (87%)	38 (13%)	4	5
1	B	317/349 (91%)	275 (87%)	42 (13%)	4	4
All	All	617/698 (88%)	537 (87%)	80 (13%)	4	4

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1105	LEU
1	A	1109	MET
1	A	1111	LEU
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	1163	ILE
1	A	1165	LYS
1	A	1168	LEU
1	A	1175	MET
1	A	1179	LYS
1	A	1181	GLU
1	A	1204	LYS
1	A	1205	THR

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Mol	Chain	Res	Type
1	A	1206	LEU
1	A	1218	LEU
1	A	1230	THR
1	A	1236	LYS
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	1292	VAL
1	A	1294	ASP
1	A	1339	VAL
1	A	1346	ILE
1	A	1354	ILE
1	A	1370	LEU
1	A	1375	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	1137	LEU
1	B	1144	THR
1	B	1157	ILE
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

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Mol	Chain	Res	Type
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	1360	VAL
1	B	1366	LYS
1	B	1367	ILE
1	B	1369	ASN
1	B	1374	LYS
1	B	1375	LEU
1	B	1392	LEU
1	B	1396	LYS
1	B	1405	VAL
1	B	1411	ASN
1	B	1440	LYS

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	1112	ASN
1	A	1202	ASN
1	A	1267	ASN
1	A	1281	ASN
1	A	1302	ASN
1	A	1334	ASN
1	A	1352	ASN
1	A	1358	GLN
1	A	1371	ASN
1	A	1407	ASN
1	A	1415	ASN
1	B	1127	ASN
1	B	1202	ASN
1	B	1267	ASN
1	B	1281	ASN
1	B	1302	ASN
1	B	1369	ASN
1	B	1407	ASN
1	B	1415	ASN

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Mol	Chain	Res	Type
1	B	1442	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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, 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	326/386 (84%)	0.64	38 (11%) 9 10	11, 32, 64, 105	33 (10%)
1	B	346/386 (89%)	0.67	41 (11%) 9 10	11, 33, 55, 80	56 (16%)
All	All	672/772 (87%)	0.66	79 (11%) 9 10	11, 33, 61, 105	89 (13%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	THR	5.2
1	B	1129	THR	5.0
1	A	1119	THR	4.7
1	B	1182	THR	4.5
1	A	1131	VAL	4.5
1	A	1265	PHE	4.4
1	B	1398	ALA	4.4
1	A	1111	LEU	4.4
1	A	1133	GLY	4.3
1	B	1133	GLY	4.3
1	A	1128	VAL	4.0
1	B	1172	SER	3.9
1	A	1175	MET	3.8
1	A	1126	VAL	3.8
1	B	1403	ALA	3.8
1	B	1113	CYS	3.6
1	A	1103	ASP	3.5
1	B	1441	ASN	3.5
1	B	1459	LEU	3.5
1	B	1128	VAL	3.4
1	A	1267	ASN	3.4
1	B	1445	TYR	3.4
1	B	1444	ARG	3.3
1	B	1216	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1105	LEU	3.2
1	A	1398	ALA	3.2
1	A	1268	SER	3.1
1	B	1132	ASN	3.1
1	B	1343	GLU	3.1
1	A	1112	ASN	3.1
1	A	1104	LEU	3.1
1	A	1366	LYS	3.1
1	A	1132	ASN	3.0
1	B	1377	PHE	2.9
1	A	1121	GLY	2.9
1	B	1134	ASP	2.8
1	B	1267	ASN	2.8
1	B	1379	PHE	2.8
1	B	1248	HIS	2.8
1	A	1266	LYS	2.7
1	A	1179	LYS	2.7
1	B	1131	VAL	2.7
1	A	1116	LEU	2.7
1	B	1369	ASN	2.6
1	A	1130	GLU	2.6
1	B	1346	ILE	2.6
1	A	1118	VAL	2.5
1	B	1399	ASN	2.5
1	A	1370	LEU	2.4
1	B	1207	TYR	2.4
1	B	1101	ASN	2.4
1	A	1206	LEU	2.4
1	B	1105	LEU	2.4
1	A	1178	PRO	2.4
1	B	1111	LEU	2.4
1	B	1252	HIS	2.4
1	A	1115	THR	2.3
1	A	1172	SER	2.3
1	B	1135	ASN	2.3
1	B	1205	THR	2.3
1	A	1216	ASP	2.2
1	B	1458	GLY	2.2
1	A	1346	ILE	2.2
1	B	1112	ASN	2.2
1	A	1347	GLU	2.2
1	B	1442	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1345	ARG	2.1
1	B	1293	VAL	2.1
1	A	1252	HIS	2.1
1	B	1141	HIS	2.1
1	A	1143	ILE	2.1
1	B	1294	ASP	2.1
1	A	1152	ARG	2.1
1	A	1157	ILE	2.1
1	A	1176	SER	2.0
1	B	1177	LEU	2.0
1	B	1181	GLU	2.0
1	B	1368	SER	2.0
1	A	1123	LEU	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 oligosaccharides 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.