



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:02 PM GMT

PDB ID : 4WOY
Title : Crystal structure and functional analysis of MiD49, a receptor for the mitochondrial fission protein Drp1
Authors : Loson, O.C.; Meng, S.; Ngo, H.B.; Liu, R.; Kaiser, J.T.; Chan, D.C.
Deposited on : 2014-10-17
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

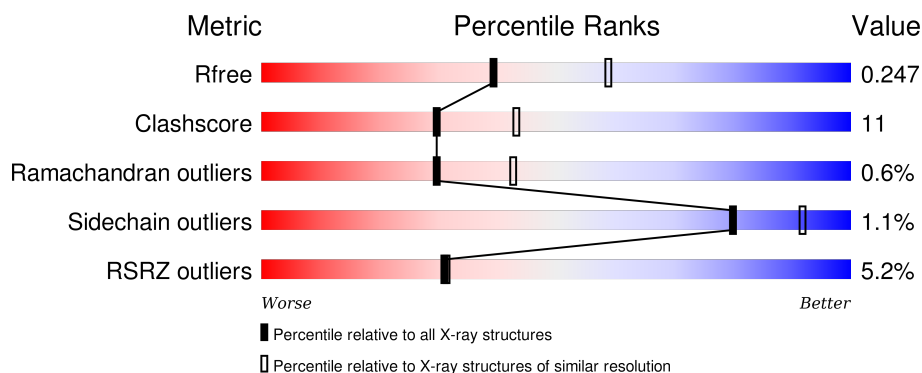
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	329	<div> <div>6%</div> <div>74%</div> <div>25%</div> </div>
1	B	329	<div> <div>4%</div> <div>82%</div> <div>17%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5337 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 Mitochondrial dynamics protein MID49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2581	1667	441	465	8			
1	B	329	Total	C	N	O	S	0	0	0
			2581	1667	441	465	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	ALA	ARG	engineered mutation	UNP Q5NCS9
B	218	ALA	ARG	engineered mutation	UNP Q5NCS9

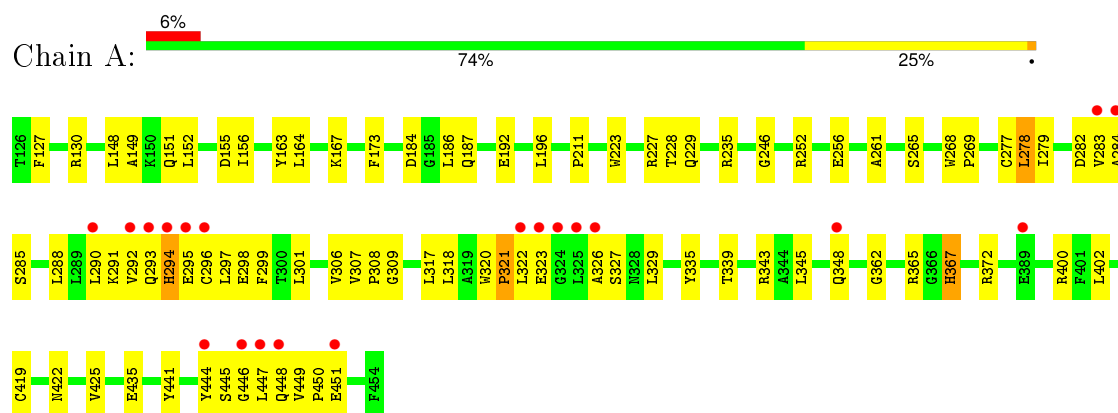
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	84	Total	O	0	0
			84	84		

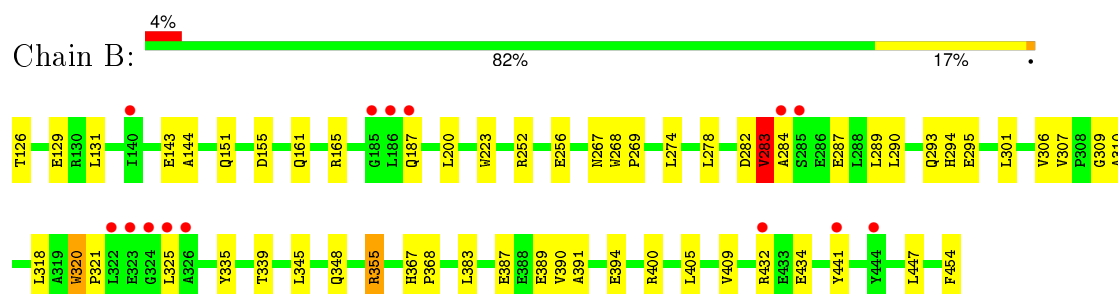
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Mitochondrial dynamics protein MID49



- Molecule 1: Mitochondrial dynamics protein MID49



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.67Å 153.39Å 109.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.98 – 2.40 36.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.98-2.40) 98.9 (36.98-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.206 , 0.243 0.217 , 0.247	Depositor DCC
R_{free} test set	904 reflections (2.82%)	DCC
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 32968 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5337	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.07 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.1759e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	1/2645 (0.0%)	0.69	1/3610 (0.0%)
1	B	0.44	0/2645	0.63	0/3610
All	All	0.47	1/5290 (0.0%)	0.66	1/7220 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	419	CYS	CB-SG	-5.32	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	LEU	N-CA-C	-7.73	90.12	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	PRO	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	2581	0	2594	71	0
1	B	2581	0	2594	48	0
2	A	91	0	0	13	0
2	B	84	0	0	13	1
All	All	5337	0	5188	116	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (116) 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:235:ARG:NH1	2:A:501:HOH:O	1.84	1.10
1:B:391:ALA:O	2:B:558:HOH:O	1.91	0.88
1:A:184:ASP:O	2:A:589:HOH:O	1.93	0.86
1:A:285:SER:N	2:A:581:HOH:O	1.95	0.85
1:A:151:GLN:NE2	1:A:155:ASP:OD2	2.13	0.82
1:A:367:HIS:ND1	2:A:502:HOH:O	2.14	0.80
1:A:343:ARG:NH2	2:A:585:HOH:O	2.14	0.80
1:A:192:GLU:OE2	2:A:590:HOH:O	2.01	0.77
1:B:187:GLN:HG2	2:B:581:HOH:O	1.84	0.76
1:A:291:LYS:HG3	1:A:292:VAL:HG22	1.67	0.76
1:B:321:PRO:O	2:B:578:HOH:O	2.07	0.71
1:A:372:ARG:NH1	1:A:435:GLU:OE2	2.23	0.71
1:A:292:VAL:HB	1:A:293:GLN:C	2.12	0.70
1:A:186:LEU:HB3	1:A:187:GLN:HG2	1.73	0.70
1:A:252:ARG:HB2	1:A:327:SER:HB3	1.73	0.69
1:A:228:THR:HG22	1:A:229:GLN:HG3	1.74	0.68
1:A:163:TYR:CE1	1:A:167:LYS:HG3	2.29	0.68
1:A:130:ARG:NH1	2:A:505:HOH:O	2.28	0.67
1:B:389:GLU:OE2	2:B:501:HOH:O	2.11	0.67
1:B:151:GLN:NE2	1:B:155:ASP:OD2	2.29	0.66
1:A:372:ARG:O	2:A:587:HOH:O	2.13	0.65
1:A:308:PRO:O	2:A:503:HOH:O	2.14	0.65
1:B:310:ALA:O	2:B:502:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:N	1:A:291:LYS:O	2.22	0.65
1:B:306:VAL:HG12	1:B:318:LEU:HD23	1.79	0.64
1:A:290:LEU:HD23	1:A:299:PHE:CE1	2.33	0.64
1:B:143:GLU:O	2:B:560:HOH:O	2.14	0.64
1:A:292:VAL:HB	1:A:294:HIS:N	2.15	0.62
1:B:131:LEU:HD12	1:B:454:PHE:HZ	1.65	0.62
1:A:292:VAL:HG12	1:A:297:LEU:O	1.99	0.62
1:A:444:TYR:CZ	1:A:445:SER:HB3	2.34	0.62
1:A:451:GLU:OE1	2:A:572:HOH:O	2.16	0.61
1:A:211:PRO:HG3	1:A:223:TRP:CH2	2.36	0.60
1:A:402:LEU:HD22	1:A:446:GLY:O	2.03	0.59
1:B:391:ALA:H	1:B:400:ARG:HH21	1.50	0.58
1:B:293:GLN:OE1	2:B:503:HOH:O	2.17	0.57
1:A:261:ALA:HA	1:A:265:SER:HB3	1.86	0.57
1:B:441:TYR:HB3	2:B:520:HOH:O	2.04	0.56
1:A:228:THR:HG22	1:A:229:GLN:N	2.19	0.56
1:B:282:ASP:O	1:B:284:ALA:N	2.39	0.56
1:A:279:ILE:HG12	1:A:290:LEU:HD13	1.87	0.56
1:A:293:GLN:O	1:A:295:GLU:N	2.39	0.55
1:B:282:ASP:OD1	1:B:283:VAL:N	2.39	0.55
1:B:161:GLN:O	1:B:165:ARG:HG3	2.07	0.55
1:A:290:LEU:HD23	1:A:299:PHE:CZ	2.41	0.55
1:A:282:ASP:OD1	1:A:283:VAL:N	2.41	0.54
1:B:223:TRP:NE1	2:B:504:HOH:O	2.31	0.53
1:B:355:ARG:HH22	1:B:394:GLU:HG3	1.74	0.53
1:A:294:HIS:O	1:A:296:CYS:N	2.40	0.53
1:A:127:PHE:CE1	1:A:450:PRO:HB2	2.43	0.53
1:B:345:LEU:O	1:B:348:GLN:HG2	2.09	0.53
1:B:309:GLY:O	2:B:533:HOH:O	2.19	0.53
1:B:335:TYR:O	1:B:339:THR:HG23	2.10	0.52
1:A:164:LEU:HD21	1:A:173:PHE:CD2	2.44	0.52
1:A:447:LEU:HB2	1:B:274:LEU:HD11	1.91	0.52
1:B:290:LEU:HB2	1:B:301:LEU:HB2	1.93	0.51
1:B:405:LEU:O	1:B:409:VAL:HG13	2.10	0.51
1:B:252:ARG:O	1:B:256:GLU:HG3	2.11	0.51
1:A:291:LYS:NZ	1:A:298:GLU:OE2	2.35	0.50
1:A:306:VAL:HG12	1:A:318:LEU:HD23	1.94	0.50
1:A:292:VAL:H	1:A:293:GLN:HA	1.76	0.49
1:A:448:GLN:HG3	1:A:449:VAL:H	1.77	0.49
1:A:448:GLN:OE1	2:A:573:HOH:O	2.18	0.49
1:A:444:TYR:CG	1:A:445:SER:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ARG:HH22	1:B:434:GLU:HB3	1.78	0.49
1:A:307:VAL:HG22	1:A:317:LEU:HB2	1.94	0.48
1:A:323:GLU:HA	1:A:327:SER:OG	2.14	0.48
1:A:345:LEU:O	1:A:348:GLN:HG2	2.13	0.48
1:A:149:ALA:HB2	1:A:297:LEU:HD21	1.96	0.48
1:B:335:TYR:CZ	1:B:339:THR:HG21	2.49	0.47
1:B:126:THR:HG23	1:B:129:GLU:H	1.79	0.47
1:A:291:LYS:HA	1:A:292:VAL:HA	1.55	0.47
1:A:246:GLY:O	2:A:501:HOH:O	2.21	0.46
1:A:372:ARG:NH1	2:A:570:HOH:O	2.25	0.46
1:B:383:LEU:O	1:B:387:GLU:HG2	2.15	0.46
1:A:279:ILE:HG12	1:A:290:LEU:CD1	2.45	0.46
1:B:282:ASP:C	1:B:284:ALA:H	2.19	0.46
1:B:223:TRP:CD1	2:B:504:HOH:O	2.69	0.46
1:A:130:ARG:HD2	1:A:451:GLU:HG2	1.98	0.46
1:B:200:LEU:HB2	1:B:307:VAL:HG12	1.96	0.46
1:A:268:TRP:N	1:A:269:PRO:HD2	2.32	0.45
1:B:432:ARG:NH2	1:B:434:GLU:HB3	2.32	0.45
1:A:441:TYR:HE1	1:B:267:ASN:HD21	1.64	0.45
1:B:390:VAL:HB	1:B:400:ARG:NH2	2.32	0.45
1:A:196:LEU:HA	1:A:196:LEU:HD12	1.84	0.45
1:B:268:TRP:N	1:B:269:PRO:HD2	2.33	0.44
1:B:290:LEU:HA	1:B:290:LEU:HD23	1.88	0.44
1:A:228:THR:HG22	1:A:229:GLN:CG	2.43	0.44
1:A:335:TYR:CZ	1:A:339:THR:HG21	2.53	0.44
1:B:294:HIS:CE1	1:B:295:GLU:HG2	2.53	0.44
1:A:290:LEU:HD12	1:A:290:LEU:HA	1.75	0.43
1:B:400:ARG:HD3	1:B:400:ARG:HA	1.67	0.43
1:A:278:LEU:O	1:A:290:LEU:HD12	2.18	0.43
1:B:282:ASP:HB3	1:B:289:LEU:HB2	2.00	0.43
1:B:325:LEU:HA	1:B:325:LEU:HD12	1.72	0.43
1:A:335:TYR:O	1:A:339:THR:HG23	2.19	0.43
1:A:326:ALA:HB1	1:A:329:LEU:HG	1.99	0.43
1:A:448:GLN:HB3	1:B:274:LEU:HA	2.00	0.42
1:B:390:VAL:HB	1:B:400:ARG:CZ	2.49	0.42
1:B:320:TRP:HD1	2:B:578:HOH:O	2.02	0.42
1:B:405:LEU:HB2	1:B:447:LEU:HD21	2.01	0.42
1:A:362:GLY:HA2	1:A:365:ARG:NH2	2.34	0.42
1:B:287:GLU:O	1:B:289:LEU:HG	2.20	0.41
1:A:288:LEU:HB2	1:A:301:LEU:HB2	2.02	0.41
1:A:277:CYS:SG	1:A:290:LEU:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:NH2	1:B:394:GLU:HG3	2.34	0.41
1:A:148:LEU:CD2	1:A:295:GLU:HG3	2.50	0.41
1:A:252:ARG:O	1:A:256:GLU:HG3	2.21	0.41
1:A:148:LEU:HD22	1:A:295:GLU:HG3	2.03	0.41
1:A:227:ARG:NH1	1:A:228:THR:O	2.54	0.41
1:A:320:TRP:CG	1:A:321:PRO:HD2	2.55	0.41
1:A:422:ASN:O	1:A:425:VAL:HG22	2.21	0.40
1:A:152:LEU:O	1:A:156:ILE:HG13	2.21	0.40
1:A:400:ARG:HA	1:A:400:ARG:HD3	1.72	0.40
1:B:367:HIS:HA	1:B:368:PRO:HD3	1.91	0.40
1:B:144:ALA:HA	2:B:560:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:HOH:O	2:B:523:HOH:O[3_856]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	327/329 (99%)	314 (96%)	10 (3%)	3 (1%)	21	30
1	B	327/329 (99%)	322 (98%)	4 (1%)	1 (0%)	46	63
All	All	654/658 (99%)	636 (97%)	14 (2%)	4 (1%)	30	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	B	283	VAL

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Mol	Chain	Res	Type
1	A	294	HIS
1	A	284	ALA

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	275/275 (100%)	273 (99%)	2 (1%)	88	95
1	B	275/275 (100%)	271 (98%)	4 (2%)	72	87
All	All	550/550 (100%)	544 (99%)	6 (1%)	80	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	LEU
1	A	367	HIS
1	B	278	LEU
1	B	283	VAL
1	B	320	TRP
1	B	355	ARG

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 [i](#)

There are no carbohydrates 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	329/329 (100%)	0.03	20 (6%) 25 25	32, 54, 122, 204	0
1	B	329/329 (100%)	-0.02	14 (4%) 39 40	34, 61, 107, 187	0
All	All	658/658 (100%)	0.00	34 (5%) 31 31	32, 57, 112, 204	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	LEU	13.5
1	A	446	GLY	11.6
1	A	389	GLU	9.1
1	B	326	ALA	7.9
1	A	296	CYS	6.4
1	B	186	LEU	6.3
1	B	323	GLU	6.2
1	A	448	GLN	6.2
1	A	324	GLY	5.9
1	A	295	GLU	5.7
1	A	294	HIS	5.7
1	A	326	ALA	5.6
1	B	284	ALA	5.6
1	A	325	LEU	5.3
1	B	441	TYR	5.0
1	A	284	ALA	4.1
1	B	185	GLY	3.9
1	B	324	GLY	3.6
1	A	451	GLU	3.5
1	B	285	SER	3.4
1	B	325	LEU	3.4
1	A	323	GLU	3.0
1	A	293	GLN	2.9
1	B	432	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	140	ILE	2.5
1	A	292	VAL	2.5
1	B	444	TYR	2.5
1	A	444	TYR	2.4
1	A	283	VAL	2.4
1	A	322	LEU	2.4
1	B	187	GLN	2.3
1	A	348	GLN	2.2
1	A	290	LEU	2.1
1	B	322	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 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.