Full wwPDB X-ray Structure Validation Report (i)

Jan 16, 2017 – 04:06 PM EST

PDB ID	:	5WTX
Title	:	Structure of Nop9
Authors	:	Ye, K.; Wang, B.
Deposited on	:	2016-12-15
Resolution	:	3.07 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

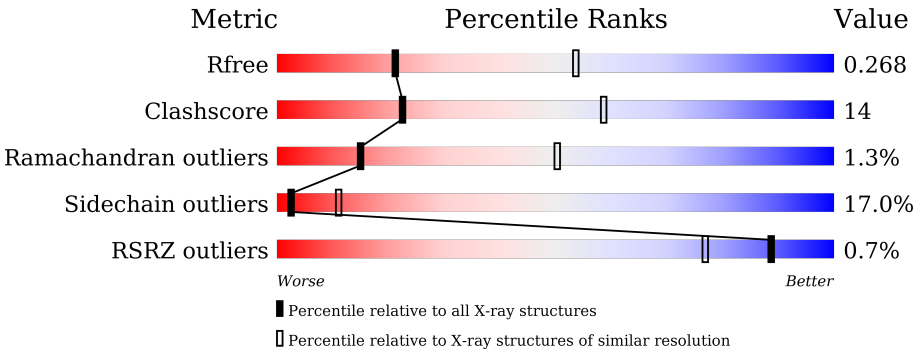
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.07 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	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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 <=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	666	% 49% 27% 6% 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4460 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.

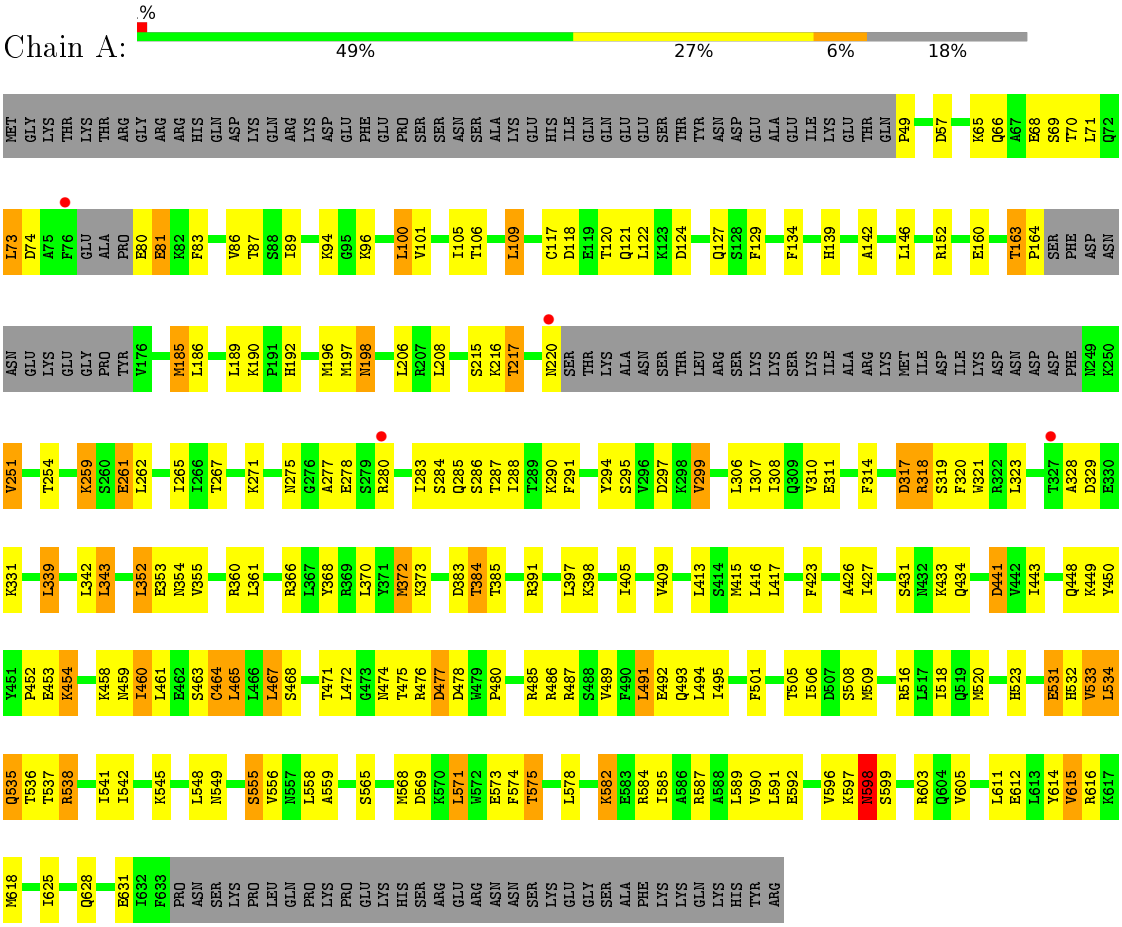
- Molecule 1 is a protein called Nucleolar protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4460	2870	745	825	20	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Nucleolar protein 9



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.80Å 134.85Å 145.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 3.07 49.52 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.52-3.07) 99.7 (49.52-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.194 , 0.266 0.195 , 0.268	Depositor DCC
R_{free} test set	891 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	72.9	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.8	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	0.94	EDS
Total number of atoms	4460	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/4541	0.63	0/6117

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	THR	Peptide
1	A	598	ASN	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	4460	0	4538	123	0
All	All	4460	0	4538	123	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 14.

All (123) 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:471:THR:HA	1:A:474:ASN:HD21	1.40	0.84
1:A:460:ILE:HD11	1:A:505:THR:HA	1.59	0.83
1:A:509:MET:HE1	1:A:533:VAL:HG11	1.60	0.83
1:A:328:ALA:HB1	1:A:329:ASP:HB2	1.66	0.78
1:A:441:ASP:OD1	1:A:441:ASP:N	2.19	0.76
1:A:368:TYR:HA	1:A:372:MET:HB2	1.67	0.75
1:A:532:HIS:O	1:A:535:GLN:NE2	2.22	0.72
1:A:186:LEU:HD13	1:A:261:GLU:HG2	1.73	0.69
1:A:321:TRP:HZ3	1:A:355:VAL:HG13	1.59	0.68
1:A:615:VAL:HG12	1:A:616:ARG:HG3	1.75	0.68
1:A:65:LYS:HE3	1:A:105:ILE:HD13	1.75	0.68
1:A:501:PHE:O	1:A:505:THR:HG23	1.95	0.67
1:A:384:THR:HG22	1:A:385:THR:HA	1.77	0.66
1:A:117:CYS:O	1:A:152:ARG:NH2	2.30	0.64
1:A:612:GLU:OE2	1:A:616:ARG:NH1	2.30	0.64
1:A:259:LYS:HG2	1:A:314:PHE:CE1	2.33	0.63
1:A:83:PHE:O	1:A:87:THR:HG23	1.99	0.62
1:A:459:ASN:HB3	1:A:461:LEU:HB2	1.83	0.61
1:A:542:ILE:HD12	1:A:542:ILE:H	1.65	0.61
1:A:460:ILE:HD12	1:A:461:LEU:N	2.17	0.59
1:A:139:HIS:HB3	1:A:142:ALA:HB3	1.83	0.59
1:A:598:ASN:O	1:A:598:ASN:ND2	2.35	0.58
1:A:531:GLU:HA	1:A:534:LEU:HD22	1.87	0.57
1:A:277:ALA:HB1	1:A:278:GLU:HA	1.86	0.57
1:A:87:THR:HB	1:A:121:GLN:HE22	1.70	0.56
1:A:405:ILE:O	1:A:409:VAL:HG23	2.06	0.56
1:A:598:ASN:HA	1:A:603:ARG:NH2	2.21	0.56
1:A:285:GLN:HA	1:A:288:ILE:HB	1.88	0.56
1:A:259:LYS:HG2	1:A:314:PHE:HE1	1.70	0.55
1:A:215:SER:OG	1:A:254:THR:HG23	2.07	0.55
1:A:308:ILE:HG21	1:A:355:VAL:HG22	1.87	0.55
1:A:558:LEU:HB3	1:A:568:MET:HG2	1.89	0.54
1:A:413:LEU:HD13	1:A:427:ILE:HD12	1.89	0.54
1:A:80:GLU:HB3	1:A:83:PHE:CE2	2.43	0.53
1:A:452:PRO:O	1:A:454:LYS:N	2.36	0.53
1:A:461:LEU:O	1:A:467:LEU:HB2	2.08	0.52
1:A:596:VAL:O	1:A:599:SER:HB3	2.09	0.52
1:A:450:TYR:HB3	1:A:460:ILE:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLU:C	1:A:575:THR:H	2.13	0.51
1:A:297:ASP:OD2	1:A:299:VAL:HG13	2.11	0.51
1:A:538:ARG:HH11	1:A:538:ARG:HG2	1.75	0.51
1:A:474:ASN:HB2	1:A:476:ARG:O	2.09	0.51
1:A:450:TYR:HD1	1:A:463:SER:HB3	1.75	0.51
1:A:475:THR:OG1	1:A:476:ARG:N	2.45	0.49
1:A:460:ILE:HD12	1:A:461:LEU:H	1.76	0.49
1:A:535:GLN:HB3	1:A:538:ARG:HB2	1.95	0.49
1:A:262:LEU:HD23	1:A:314:PHE:CE2	2.48	0.49
1:A:285:GLN:H	1:A:285:GLN:CD	2.17	0.48
1:A:311:GLU:OE2	1:A:320:PHE:HB2	2.12	0.48
1:A:575:THR:HG21	1:A:582:LYS:HG3	1.96	0.48
1:A:217:THR:HA	1:A:251:VAL:HG13	1.96	0.48
1:A:267:THR:O	1:A:271:LYS:HG2	2.14	0.47
1:A:480:PRO:HB3	1:A:523:HIS:CE1	2.49	0.47
1:A:460:ILE:HA	1:A:463:SER:HB2	1.96	0.47
1:A:571:LEU:O	1:A:575:THR:HB	2.15	0.47
1:A:506:ILE:HA	1:A:509:MET:CE	2.45	0.47
1:A:284:SER:OG	1:A:287:THR:HG23	2.14	0.46
1:A:192:HIS:O	1:A:196:MET:HG3	2.15	0.46
1:A:69:SER:O	1:A:73:LEU:HD23	2.16	0.46
1:A:342:LEU:HD13	1:A:352:LEU:HG	1.98	0.46
1:A:464:CYS:O	1:A:487:ARG:HD2	2.15	0.46
1:A:353:GLU:HG3	1:A:354:ASN:N	2.30	0.46
1:A:556:VAL:HG22	1:A:589:LEU:HD23	1.97	0.46
1:A:459:ASN:ND2	1:A:508:SER:HB3	2.30	0.46
1:A:49:PRO:HD3	1:A:134:PHE:CE2	2.51	0.45
1:A:66:GLN:O	1:A:69:SER:OG	2.28	0.45
1:A:73:LEU:O	1:A:74:ASP:HB2	2.17	0.45
1:A:471:THR:CA	1:A:474:ASN:HD21	2.20	0.45
1:A:476:ARG:O	1:A:478:ASP:N	2.47	0.45
1:A:198:ASN:N	1:A:198:ASN:OD1	2.47	0.45
1:A:311:GLU:OE1	1:A:318:ARG:HB3	2.17	0.45
1:A:339:LEU:O	1:A:343:LEU:HD22	2.17	0.45
1:A:397:LEU:O	1:A:398:LYS:HD3	2.17	0.45
1:A:548:LEU:HD12	1:A:578:LEU:HD23	1.99	0.44
1:A:317:ASP:OD1	1:A:318:ARG:HA	2.18	0.44
1:A:423:PHE:O	1:A:426:ALA:HB3	2.16	0.44
1:A:68:GLU:HB2	1:A:109:LEU:HG	1.99	0.44
1:A:485:ARG:O	1:A:489:VAL:HG23	2.17	0.44
1:A:571:LEU:HA	1:A:574:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ALA:HB1	1:A:278:GLU:CA	2.48	0.44
1:A:287:THR:HA	1:A:290:LYS:HB2	2.00	0.44
1:A:468:SER:HA	1:A:516:ARG:NH2	2.33	0.44
1:A:307:ILE:HA	1:A:310:VAL:HG12	2.00	0.44
1:A:495:ILE:O	1:A:538:ARG:NH2	2.48	0.44
1:A:468:SER:HA	1:A:516:ARG:HH21	1.84	0.43
1:A:261:GLU:O	1:A:265:ILE:HG23	2.19	0.43
1:A:160:GLU:O	1:A:164:PRO:HD3	2.18	0.43
1:A:578:LEU:HD12	1:A:578:LEU:HA	1.79	0.43
1:A:383:ASP:HA	1:A:384:THR:HA	1.77	0.43
1:A:185:MET:HE1	1:A:186:LEU:HD23	2.00	0.43
1:A:101:VAL:HG21	1:A:129:PHE:CZ	2.54	0.43
1:A:465:LEU:HD21	1:A:491:LEU:HD12	2.00	0.42
1:A:492:GLU:O	1:A:495:ILE:HB	2.19	0.42
1:A:94:LYS:HB2	1:A:94:LYS:HE2	1.87	0.42
1:A:373:LYS:HE3	1:A:373:LYS:HB2	1.92	0.42
1:A:545:LYS:HG3	1:A:578:LEU:HD21	2.02	0.42
1:A:559:ALA:HB1	1:A:605:VAL:HG21	2.00	0.42
1:A:472:LEU:HB3	1:A:516:ARG:NH1	2.34	0.42
1:A:518:ILE:HD12	1:A:518:ILE:HG23	1.82	0.42
1:A:100:LEU:HD23	1:A:106:THR:HB	2.01	0.42
1:A:189:LEU:O	1:A:192:HIS:N	2.44	0.42
1:A:398:LYS:HD3	1:A:398:LYS:HA	1.67	0.42
1:A:86:VAL:O	1:A:89:ILE:HB	2.20	0.42
1:A:384:THR:CG2	1:A:385:THR:HA	2.49	0.42
1:A:291:PHE:O	1:A:294:TYR:HB2	2.20	0.41
1:A:317:ASP:OD1	1:A:317:ASP:N	2.42	0.41
1:A:317:ASP:HB2	1:A:319:SER:N	2.34	0.41
1:A:383:ASP:HA	1:A:384:THR:HG23	2.02	0.41
1:A:509:MET:HB2	1:A:509:MET:HE3	1.98	0.41
1:A:555:SER:OG	1:A:585:ILE:HG12	2.20	0.41
1:A:590:VAL:HG21	1:A:614:TYR:CD1	2.54	0.41
1:A:96:LYS:HB2	1:A:100:LEU:HD12	2.02	0.41
1:A:518:ILE:HD13	1:A:518:ILE:HA	1.83	0.41
1:A:81:GLU:O	1:A:81:GLU:HG2	2.20	0.41
1:A:366:ARG:O	1:A:370:LEU:HB2	2.20	0.41
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.81	0.41
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.88	0.41
1:A:582:LYS:HD3	1:A:625:ILE:CD1	2.51	0.41
1:A:458:LYS:O	1:A:459:ASN:C	2.59	0.40
1:A:509:MET:CE	1:A:533:VAL:HG11	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:GLU:C	1:A:575:THR:N	2.75	0.40
1:A:461:LEU:HD11	1:A:509:MET:HG2	2.03	0.40
1:A:416:LEU:HD23	1:A:416:LEU:HA	1.78	0.40

There are no symmetry-related clashes.

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	535/666 (80%)	485 (91%)	43 (8%)	7 (1%)	15 50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	THR
1	A	275	ASN
1	A	295	SER
1	A	57	ASP
1	A	477	ASP
1	A	453	GLU
1	A	618	MET

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	500/613 (82%)	415 (83%)	85 (17%)	2 11

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	71	LEU
1	A	73	LEU
1	A	81	GLU
1	A	100	LEU
1	A	109	LEU
1	A	118	ASP
1	A	120	THR
1	A	122	LEU
1	A	124	ASP
1	A	127	GLN
1	A	146	LEU
1	A	185	MET
1	A	190	LYS
1	A	197	MET
1	A	198	ASN
1	A	206	LEU
1	A	208	LEU
1	A	216	LYS
1	A	217	THR
1	A	220	ASN
1	A	251	VAL
1	A	259	LYS
1	A	261	GLU
1	A	280	ARG
1	A	283	ILE
1	A	286	SER
1	A	299	VAL
1	A	306	LEU
1	A	317	ASP
1	A	318	ARG
1	A	323	LEU
1	A	331	LYS
1	A	339	LEU
1	A	343	LEU
1	A	352	LEU
1	A	360	ARG
1	A	361	LEU

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Mol	Chain	Res	Type
1	A	372	MET
1	A	384	THR
1	A	391	ARG
1	A	415	MET
1	A	417	LEU
1	A	431	SER
1	A	433	LYS
1	A	434	GLN
1	A	441	ASP
1	A	443	ILE
1	A	448	GLN
1	A	449	LYS
1	A	454	LYS
1	A	460	ILE
1	A	464	CYS
1	A	465	LEU
1	A	467	LEU
1	A	477	ASP
1	A	486	ARG
1	A	491	LEU
1	A	493	GLN
1	A	494	LEU
1	A	520	MET
1	A	531	GLU
1	A	533	VAL
1	A	534	LEU
1	A	535	GLN
1	A	536	THR
1	A	537	THR
1	A	538	ARG
1	A	541	ILE
1	A	549	ASN
1	A	555	SER
1	A	565	SER
1	A	569	ASP
1	A	571	LEU
1	A	575	THR
1	A	582	LYS
1	A	584	ARG
1	A	587	ARG
1	A	591	LEU
1	A	592	GLU

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Mol	Chain	Res	Type
1	A	597	LYS
1	A	598	ASN
1	A	615	VAL
1	A	628	GLN
1	A	631	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	474	ASN
1	A	493	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	543/666 (81%)	-0.03	4 (0%)	89	77	44, 64, 93, 124	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	PHE	3.3
1	A	327	THR	2.4
1	A	220	ASN	2.2
1	A	280	ARG	2.2

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.