Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 01:52 AM EST

PDB ID	:	1PJR
Title	:	STRUCTURE OF DNA HELICASE
Authors	:	Subramanya, H.S.; Bird, L.E.; Brannigan, J.A.; Wigley, D.B.
Deposited on	:	1996-10-11
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

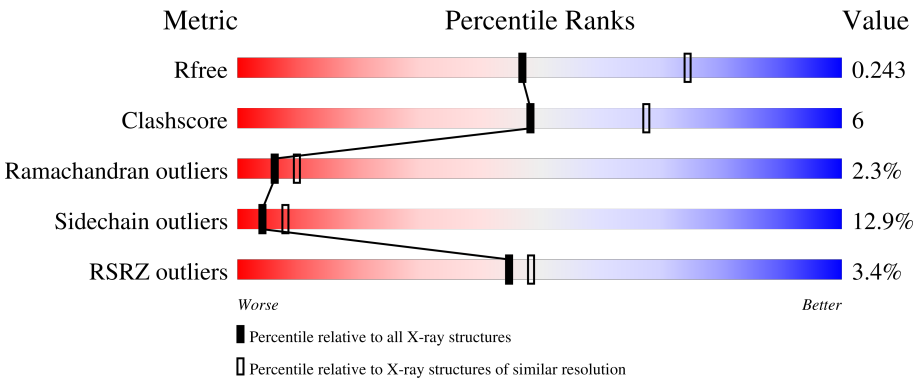
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	724	3% 61% 20% 5% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5278 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 PCRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	623	5053	3200	884	949	20	0	0	0

- Molecule 2 is water.

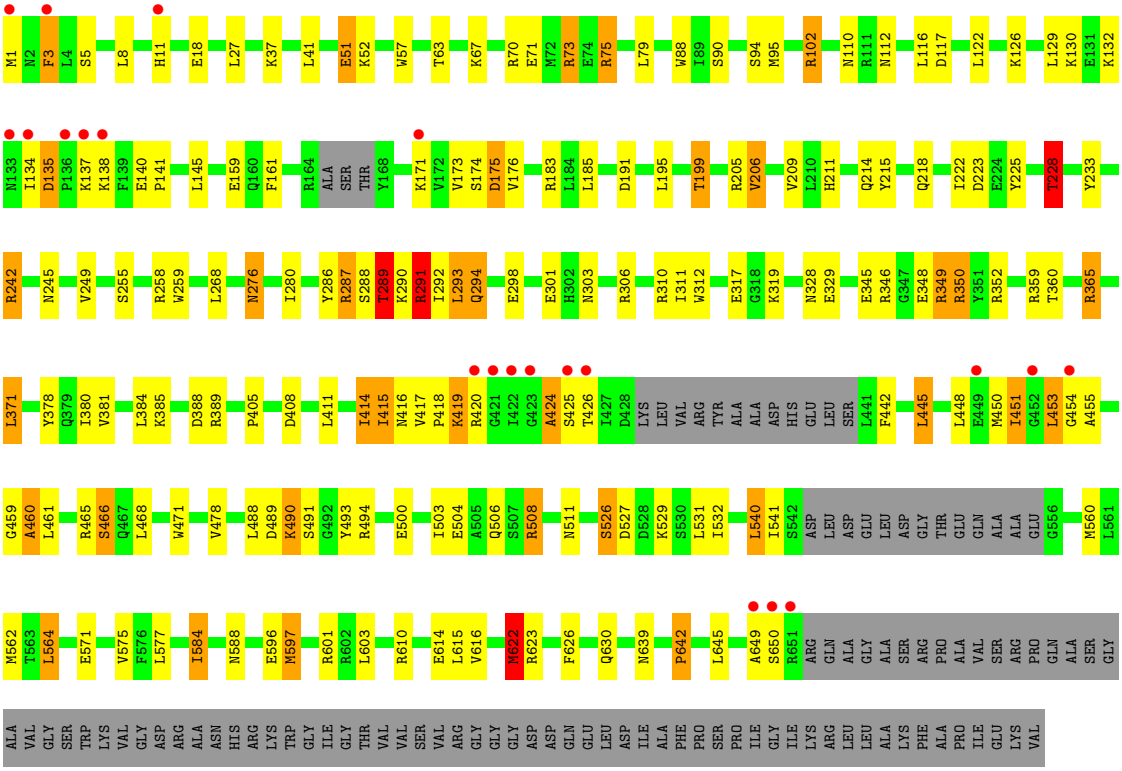
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	225	225	225	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PCRA

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	139.06Å 139.06Å 111.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 96.7 (10.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.16 (at 2.50Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , 0.269 0.197 , 0.243	Depositor DCC
R_{free} test set	1990 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 81.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5278	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 (i)

5.1 Standard geometry (i)

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	0.77	0/5139	1.48	57/6936 (0.8%)

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

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	A	137	LYS	CA-C-N	-10.85	93.33	117.20
1	A	597	MET	CG-SD-CE	-9.71	84.66	100.20
1	A	233	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	A	75	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	A	88	TRP	CD1-CG-CD2	7.98	112.69	106.30
1	A	312	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	A	425	SER	N-CA-C	7.94	132.43	111.00
1	A	57	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	A	465	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	259	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	A	312	TRP	CE2-CD2-CG	-7.41	101.38	107.30
1	A	73	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	137	LYS	O-C-N	7.24	134.28	122.70
1	A	57	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	A	259	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	306	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	88	TRP	CE2-CD2-CG	-7.11	101.61	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	THR	N-CA-CB	-7.10	96.81	110.30
1	A	471	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	A	426	THR	N-CA-C	-6.82	92.58	111.00
1	A	73	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	191	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	291	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	359	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	623	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	287	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	137	LYS	CA-CB-CG	-6.46	99.18	113.40
1	A	471	TRP	CE2-CD2-CG	-6.41	102.17	107.30
1	A	205	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	365	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	350	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	623	ARG	CA-CB-CG	6.09	126.80	113.40
1	A	228	THR	N-CA-CB	-5.97	98.96	110.30
1	A	411	LEU	CA-CB-CG	5.88	128.84	115.30
1	A	575	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	A	310	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	448	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	95	MET	CA-CB-CG	5.66	122.92	113.30
1	A	508	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	415	ILE	CB-CA-C	-5.56	100.48	111.60
1	A	425	SER	N-CA-CB	-5.53	102.21	110.50
1	A	650	SER	N-CA-C	-5.48	96.19	111.00
1	A	564	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	560	MET	CG-SD-CE	-5.29	91.74	100.20
1	A	419	LYS	N-CA-C	-5.27	96.77	111.00
1	A	388	ASP	CA-CB-CG	5.22	124.89	113.40
1	A	622	MET	CA-CB-CG	5.22	122.17	113.30
1	A	508	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	51	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	A	258	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	312	TRP	CG-CD2-CE3	5.09	138.49	133.90
1	A	310	ARG	CB-CG-CD	-5.09	98.36	111.60
1	A	466	SER	N-CA-CB	-5.07	102.90	110.50
1	A	286	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	A	102	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	350	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5053	0	5068	61	0
2	A	225	0	0	5	0
All	All	5278	0	5068	61	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 6.

All (61) 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:287:ARG:HD3	1:A:571:GLU:HB3	1.58	0.86
1:A:584:ILE:HD11	1:A:630:GLN:HE22	1.55	0.72
1:A:291:ARG:HG3	1:A:645:LEU:HD22	1.72	0.71
1:A:214:GLN:HB3	1:A:242:ARG:HG2	1.76	0.66
1:A:328:ASN:HA	1:A:622:MET:O	1.98	0.64
1:A:389:ARG:HH11	1:A:511:ASN:HD21	1.46	0.64
1:A:424:ALA:HB1	1:A:460:ALA:HA	1.79	0.63
1:A:289:THR:HG21	2:A:769:HOH:O	1.99	0.61
1:A:451:ILE:HB	1:A:453:LEU:HD23	1.83	0.61
1:A:173:VAL:HA	1:A:176:VAL:HG12	1.84	0.59
1:A:564:LEU:HB3	1:A:603:LEU:HD22	1.83	0.59
1:A:27:LEU:HD11	1:A:280:ILE:HD12	1.85	0.58
1:A:71:GLU:O	1:A:75:ARG:HD2	2.04	0.56
1:A:289:THR:HG22	1:A:292:ILE:H	1.71	0.55
1:A:37:LYS:HE2	1:A:223:ASP:OD1	2.07	0.54
1:A:298:GLU:HG3	1:A:642:PRO:HG3	1.88	0.54
1:A:526:SER:O	1:A:529:LYS:HE2	2.08	0.54
1:A:532:ILE:H	1:A:532:ILE:HD12	1.73	0.53
1:A:1:MET:H2	1:A:51:GLU:CD	2.11	0.53
1:A:288:SER:HB2	1:A:293:LEU:HD13	1.93	0.51
1:A:132:LYS:NZ	1:A:175:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:PRO:HG2	1:A:420:ARG:HG3	1.93	0.49
1:A:3:PHE:H	1:A:3:PHE:HD1	1.62	0.48
1:A:195:LEU:O	1:A:199:THR:HG23	2.14	0.48
1:A:350:ARG:HD2	1:A:352:ARG:HH11	1.78	0.48
1:A:385:LYS:NZ	2:A:842:HOH:O	2.47	0.47
1:A:255:SER:HB2	2:A:760:HOH:O	2.14	0.47
1:A:381:VAL:HB	1:A:562:MET:HB3	1.97	0.47
1:A:287:ARG:NH1	1:A:571:GLU:HG2	2.30	0.47
1:A:211:HIS:O	1:A:215:TYR:HD1	1.98	0.47
1:A:319:LYS:HD2	1:A:614:GLU:HG2	1.97	0.47
1:A:303:ASN:ND2	1:A:601:ARG:HE	2.13	0.46
1:A:504:GLU:O	1:A:508:ARG:HG3	2.16	0.46
1:A:290:LYS:HB2	1:A:317:GLU:HA	1.99	0.45
1:A:289:THR:HG23	1:A:317:GLU:O	2.16	0.44
1:A:489:ASP:OD1	1:A:490:LYS:NZ	2.50	0.44
1:A:130:LYS:HD2	2:A:944:HOH:O	2.17	0.43
1:A:110:ASN:HB3	1:A:112:ASN:ND2	2.34	0.43
1:A:161:PHE:HD2	1:A:174:SER:HB3	1.83	0.43
1:A:584:ILE:HD11	1:A:630:GLN:NE2	2.26	0.43
1:A:5:SER:HA	1:A:8:LEU:HD12	2.00	0.43
1:A:294:GLN:HG3	1:A:645:LEU:HD11	2.01	0.42
1:A:41:LEU:HD13	1:A:249:VAL:HG21	2.00	0.42
1:A:491:SER:OG	1:A:493:TYR:HB2	2.19	0.42
1:A:90:SER:HB2	1:A:94:SER:HB2	2.00	0.42
1:A:445:LEU:HD11	1:A:461:LEU:HD22	2.01	0.42
1:A:242:ARG:HH11	1:A:242:ARG:HD3	1.71	0.42
1:A:225:TYR:O	1:A:228:THR:HB	2.20	0.42
1:A:348:GLU:O	1:A:349:ARG:HD3	2.19	0.42
1:A:276:ASN:ND2	1:A:276:ASN:H	2.17	0.41
1:A:206:VAL:HG22	1:A:209:VAL:HG23	2.02	0.41
1:A:371:LEU:HD12	1:A:378:TYR:HB3	2.03	0.41
1:A:122:LEU:O	1:A:126:LYS:HE2	2.20	0.41
1:A:291:ARG:HB2	1:A:317:GLU:O	2.21	0.41
1:A:140:GLU:HA	1:A:141:PRO:HD2	1.87	0.41
1:A:414:ILE:HA	1:A:417:VAL:HG12	2.03	0.41
1:A:218:GLN:O	1:A:245:ASN:HB2	2.20	0.41
1:A:405:PRO:O	1:A:442:PHE:HB2	2.21	0.41
1:A:102:ARG:NH1	2:A:814:HOH:O	2.53	0.40
1:A:311:ILE:HD13	1:A:311:ILE:HG21	1.75	0.40
1:A:424:ALA:HB1	1:A:460:ALA:CA	2.48	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	615/724 (85%)	572 (93%)	29 (5%)	14 (2%)	6 10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	ASP
1	A	453	LEU
1	A	455	ALA
1	A	346	ARG
1	A	424	ALA
1	A	454	GLY
1	A	649	ALA
1	A	11	HIS
1	A	138	LYS
1	A	460	ALA
1	A	540	LEU
1	A	134	ILE
1	A	459	GLY
1	A	541	ILE

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	542/618 (88%)	472 (87%)	70 (13%)	4 8

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	18	GLU
1	A	52	LYS
1	A	63	THR
1	A	67	LYS
1	A	70	ARG
1	A	73	ARG
1	A	79	LEU
1	A	116	LEU
1	A	117	ASP
1	A	129	LEU
1	A	145	LEU
1	A	159	GLU
1	A	171	LYS
1	A	175	ASP
1	A	183	ARG
1	A	185	LEU
1	A	199	THR
1	A	206	VAL
1	A	222	ILE
1	A	228	THR
1	A	242	ARG
1	A	268	LEU
1	A	276	ASN
1	A	289	THR
1	A	291	ARG
1	A	293	LEU
1	A	294	GLN
1	A	301	GLU
1	A	329	GLU
1	A	345	GLU
1	A	349	ARG
1	A	360	THR
1	A	365	ARG
1	A	371	LEU
1	A	380	ILE
1	A	384	LEU
1	A	408	ASP
1	A	414	ILE
1	A	415	ILE
1	A	416	ASN
1	A	419	LYS
1	A	445	LEU

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Mol	Chain	Res	Type
1	A	450	MET
1	A	451	ILE
1	A	466	SER
1	A	468	LEU
1	A	478	VAL
1	A	488	LEU
1	A	490	LYS
1	A	494	ARG
1	A	500	GLU
1	A	503	ILE
1	A	506	GLN
1	A	526	SER
1	A	527	ASP
1	A	531	LEU
1	A	540	LEU
1	A	577	LEU
1	A	584	ILE
1	A	588	ASN
1	A	596	GLU
1	A	597	MET
1	A	610	ARG
1	A	615	LEU
1	A	616	VAL
1	A	622	MET
1	A	626	PHE
1	A	639	ASN
1	A	642	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	66	ASN
1	A	112	ASN
1	A	214	GLN
1	A	276	ASN
1	A	303	ASN
1	A	315	ASN
1	A	379	GLN
1	A	416	ASN
1	A	511	ASN
1	A	524	ASN

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Mol	Chain	Res	Type
1	A	630	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	623/724 (86%)	-0.67	21 (3%) 45 48	11, 30, 83, 130	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	GLY	6.3
1	A	11	HIS	4.8
1	A	650	SER	4.7
1	A	420	ARG	4.3
1	A	133	ASN	4.0
1	A	454	GLY	3.3
1	A	423	GLY	3.2
1	A	422	ILE	3.2
1	A	1	MET	3.2
1	A	138	LYS	3.1
1	A	136	PRO	3.0
1	A	649	ALA	3.0
1	A	134	ILE	2.8
1	A	426	THR	2.7
1	A	425	SER	2.6
1	A	137	LYS	2.5
1	A	452	GLY	2.3
1	A	449	GLU	2.2
1	A	171	LYS	2.2
1	A	651	ARG	2.1
1	A	3	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.