W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	1F9U
Title	:	CRYSTAL STRUCTURES OF MUTANTS REVEAL A SIGNALLING PATHWAY FOR ACTIVATION OF THE KINESIN MOTOR ATPASE
Authors	:	Yun, M.; Zhang, X.; Park, C.G.; Park, H.W.; Endow, S.A.
Deposited on	:	2000-07-11
Resolution	:	1.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
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 1.70 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	Percentile Ranks	Value
Rfree		0.240
Clashscore		15
Ramachandran outliers		1.0%
Sidechain outliers		12.8%
RSRZ outliers		7.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
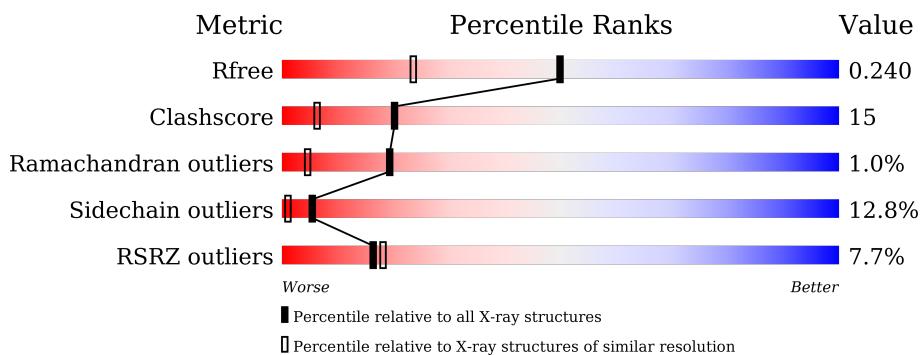
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	347	7% 57% 27% 6% 11%
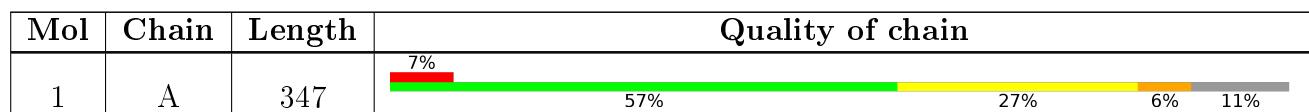
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2680 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 KINESIN-LIKE PROTEIN KAR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2443	1527	427	480	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	MET	LYS	ENGINEERED	UNP P17119
A	650	LYS	ASN	ENGINEERED	UNP P17119

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
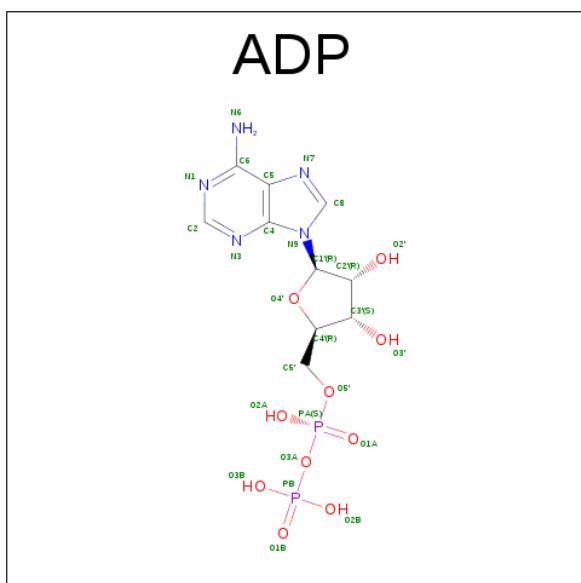
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total 209	O 209	0	0

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: KINESIN-LIKE PROTEIN KAR3
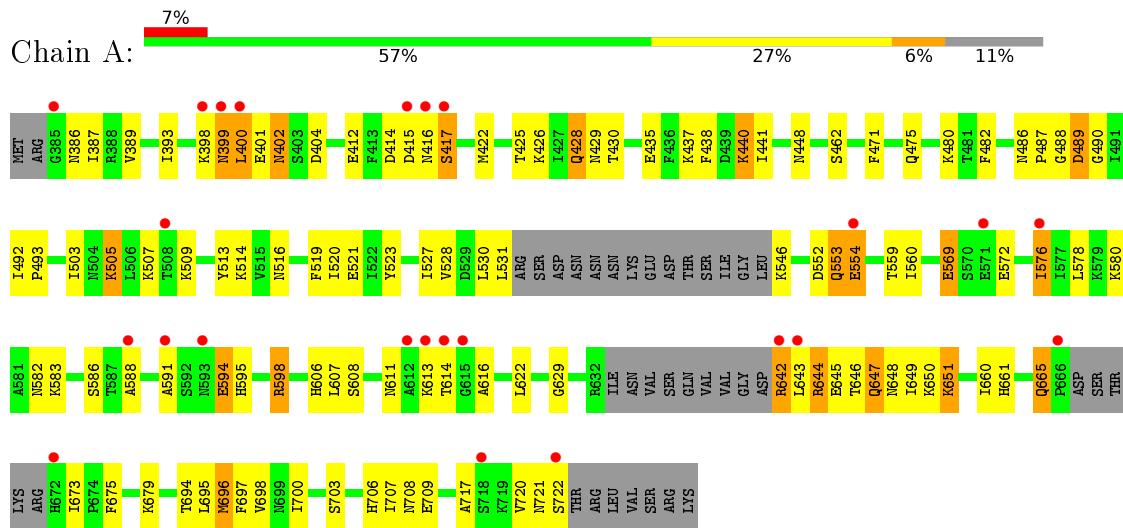
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.57Å 78.04Å 47.27Å 90.00° 105.07° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.61 – 1.50	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-1.70) 71.0 (19.61-1.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.50Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.217 , 0.266 0.195 , 0.240	Depositor DCC
R_{free} test set	2817 reflections (10.19%)	DCC
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2680	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	0.36	0/2481	0.58	0/3347

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2443	0	2422	72	0
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	209	0	0	4	0
All	All	2680	0	2434	72	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 15.

All (72) 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:426:LYS:HB3	1:A:428:GLN:HE22	1.20	1.01
1:A:698:VAL:HG21	1:A:717:ALA:HB2	1.46	0.95
1:A:598:ARG:HH11	1:A:649:ILE:HD13	1.39	0.88
1:A:393:ILE:HG12	1:A:700:ILE:HD11	1.65	0.79
1:A:402:ASN:HD22	1:A:404:ASP:H	1.29	0.79
1:A:426:LYS:HB3	1:A:428:GLN:NE2	1.98	0.77
1:A:594:GLU:HB2	4:A:119:HOH:O	1.90	0.71
1:A:402:ASN:ND2	1:A:404:ASP:H	1.90	0.70
1:A:698:VAL:HG21	1:A:717:ALA:CB	2.24	0.67
1:A:401:GLU:HB3	1:A:703:SER:OG	1.95	0.67
1:A:475:GLN:HE22	1:A:706:HIS:HB3	1.58	0.67
1:A:428:GLN:H	1:A:428:GLN:CD	2.00	0.66
1:A:389:VAL:HG21	1:A:721:ASN:HB3	1.82	0.62
1:A:614:THR:HG22	1:A:616:ALA:H	1.68	0.58
1:A:696:MET:HA	1:A:696:MET:HE2	1.86	0.58
1:A:553:GLN:HG3	4:A:232:HOH:O	2.04	0.58
1:A:588:ALA:HB3	1:A:591:ALA:HB2	1.85	0.57
1:A:492:ILE:HB	1:A:493:PRO:HD3	1.86	0.57
1:A:414:ASP:OD1	1:A:417:SER:HB2	2.04	0.57
1:A:519:PHE:HB3	1:A:531:LEU:HG	1.87	0.56
1:A:398:LYS:O	1:A:399:ASN:HB2	2.04	0.56
1:A:471:PHE:HB2	1:A:696:MET:HE2	1.89	0.55
1:A:435:GLU:OE1	1:A:437:LYS:HE3	2.08	0.53
1:A:448:ASN:HD22	1:A:489:ASP:HB3	1.73	0.53
1:A:426:LYS:NZ	1:A:708:ASN:HD21	2.06	0.53
1:A:462:SER:HB3	1:A:607:LEU:HD12	1.90	0.53
1:A:673:ILE:HB	1:A:675:PHE:CE2	2.45	0.52
1:A:552:ASP:OD2	1:A:554:GLU:HB3	2.09	0.51
1:A:425:THR:CG2	1:A:430:THR:HA	2.41	0.51
1:A:493:PRO:HG3	1:A:578:LEU:HD13	1.93	0.50
1:A:521:GLU:HG2	1:A:528:VAL:HB	1.93	0.50
1:A:503:ILE:HG12	1:A:513:TYR:HB2	1.94	0.49
1:A:402:ASN:HD22	1:A:402:ASN:C	2.14	0.49
1:A:401:GLU:HB3	1:A:703:SER:CB	2.43	0.48
1:A:709:GLU:HA	1:A:709:GLU:OE1	2.12	0.48
1:A:505:LYS:O	1:A:505:LYS:HG3	2.14	0.48
1:A:642:ARG:NH1	1:A:642:ARG:HG2	2.29	0.48
1:A:611:ASN:CG	1:A:614:THR:HB	2.34	0.48
1:A:438:PHE:HE1	1:A:717:ALA:HB1	1.78	0.48
1:A:462:SER:OG	1:A:622:LEU:HG	2.14	0.47
1:A:422:MET:HB3	1:A:441:ILE:HD13	1.98	0.46
1:A:527:ILE:HG13	1:A:679:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:O	1:A:486:ASN:HB2	2.15	0.46
1:A:516:ASN:ND2	1:A:606:HIS:HB2	2.29	0.46
1:A:661:HIS:NE2	1:A:665:GLN:OE1	2.48	0.46
1:A:642:ARG:HH11	1:A:642:ARG:CG	2.29	0.45
1:A:480:LYS:HE2	1:A:480:LYS:HB2	1.74	0.45
1:A:598:ARG:HD3	1:A:649:ILE:HD13	1.99	0.45
1:A:487:PRO:C	1:A:489:ASP:H	2.21	0.45
1:A:645:GLU:O	1:A:648:ASN:HB2	2.16	0.45
1:A:402:ASN:C	1:A:402:ASN:ND2	2.70	0.45
1:A:582:ASN:O	1:A:586:SER:HB2	2.17	0.44
1:A:644:ARG:HB3	1:A:644:ARG:HE	1.71	0.44
1:A:720:VAL:CG1	1:A:720:VAL:O	2.65	0.44
1:A:569:GLU:HG3	4:A:10:HOH:O	2.17	0.43
1:A:613:LYS:CG	1:A:614:THR:N	2.80	0.43
1:A:471:PHE:HB2	1:A:696:MET:CE	2.48	0.43
1:A:514:LYS:NZ	4:A:234:HOH:O	2.52	0.43
1:A:647:GLN:HA	1:A:647:GLN:NE2	2.33	0.43
1:A:660:ILE:HD12	1:A:694:THR:HG21	2.01	0.43
1:A:559:THR:CG2	1:A:560:ILE:N	2.82	0.42
1:A:426:LYS:HE3	1:A:707:ILE:CG2	2.49	0.42
1:A:521:GLU:HB3	1:A:530:LEU:HD11	2.01	0.42
1:A:651:LYS:HA	1:A:651:LYS:HE3	2.02	0.41
1:A:572:GLU:O	1:A:576:ILE:HG12	2.20	0.41
1:A:428:GLN:NE2	1:A:428:GLN:H	2.18	0.41
1:A:400:LEU:HD23	1:A:400:LEU:HA	1.88	0.41
1:A:598:ARG:HH22	1:A:629:GLY:HA3	1.86	0.41
1:A:523:TYR:CD2	1:A:595:HIS:HE1	2.38	0.41
1:A:440:LYS:HG3	1:A:441:ILE:N	2.36	0.41
1:A:646:THR:HG22	1:A:650:LYS:HD3	2.04	0.40
1:A:516:ASN:HD21	1:A:606:HIS:HB2	1.85	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	302/347 (87%)	293 (97%)	6 (2%)	3 (1%)	19 4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	ASN
1	A	490	GLY
1	A	488	GLY

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	282/317 (89%)	246 (87%)	36 (13%)	5 1

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	ASN
1	A	387	ILE
1	A	399	ASN
1	A	400	LEU
1	A	402	ASN
1	A	412	GLU
1	A	415	ASP
1	A	416	ASN
1	A	417	SER
1	A	428	GLN
1	A	440	LYS
1	A	489	ASP
1	A	505	LYS
1	A	507	LYS
1	A	509	LYS
1	A	520	ILE

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Mol	Chain	Res	Type
1	A	546	LYS
1	A	553	GLN
1	A	554	GLU
1	A	569	GLU
1	A	576	ILE
1	A	580	LYS
1	A	583	LYS
1	A	594	GLU
1	A	598	ARG
1	A	608	SER
1	A	642	ARG
1	A	643	LEU
1	A	644	ARG
1	A	647	GLN
1	A	651	LYS
1	A	665	GLN
1	A	695	LEU
1	A	696	MET
1	A	697	PHE
1	A	722	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	ASN
1	A	428	GLN
1	A	475	GLN
1	A	516	ASN
1	A	526	ASN
1	A	672	HIS
1	A	685	GLN
1	A	708	ASN

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)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	ADP	A	999	2	24,29,29	1.19	4 (16%)	23,45,45	2.81	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	999	2	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ADP	C5-N7	-2.18	1.31	1.39
3	A	999	ADP	PA-O2A	-2.14	1.46	1.55
3	A	999	ADP	O4'-C1'	2.24	1.44	1.41
3	A	999	ADP	PB-O2B	2.25	1.62	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ADP	N3-C2-N1	-12.59	118.98	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	310/347 (89%)	0.11	24 (7%)	16	18	8, 19, 53, 70	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	642	ARG	5.3
1	A	612	ALA	4.5
1	A	399	ASN	4.4
1	A	385	GLY	3.7
1	A	417	SER	3.6
1	A	593	ASN	3.5
1	A	613	LYS	3.5
1	A	400	LEU	3.1
1	A	672	HIS	3.1
1	A	614	THR	3.0
1	A	643	LEU	2.9
1	A	591	ALA	2.8
1	A	722	SER	2.8
1	A	416	ASN	2.7
1	A	588	ALA	2.6
1	A	398	LYS	2.5
1	A	576	ILE	2.4
1	A	415	ASP	2.3
1	A	666	PRO	2.3
1	A	718	SER	2.2
1	A	554	GLU	2.2
1	A	615	GLY	2.1
1	A	571	GLU	2.0
1	A	508	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	ADP	A	999	27/27	0.97	0.07	-0.39	7,13,17,21	0
2	MG	A	997	1/1	0.97	0.14	-	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.