wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 03:59 AM EDT

PDB ID	:	1K8K
Title	:	Crystal Structure of Arp2/3 Complex
Authors	:	Robinson, R.C.; Turbedsky, K.; Kaiser, D.A.; Higgs, H.N.; Marchand, J.-B.; Choe, S.; Pollard, T.D.
Deposited on	:	2001-10-24
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

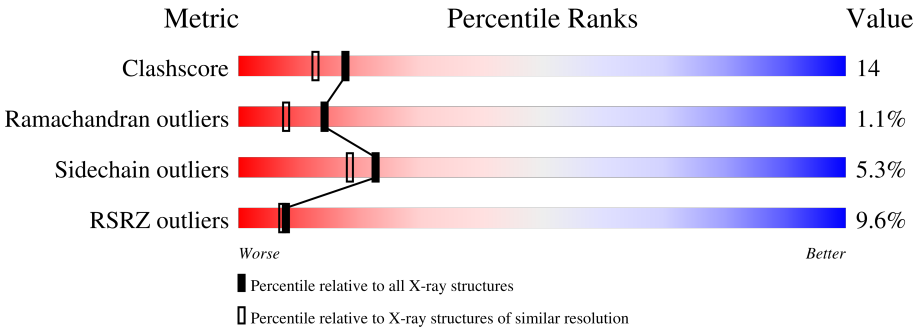
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	418	8% 78% 14%
2	B	394	10% 31% 14% 52%
3	C	372	8% 74% 18% 5%
4	D	300	2% 80% 13% 5%
5	E	178	12% 62% 28% 7%
6	F	168	4% 85% 14%

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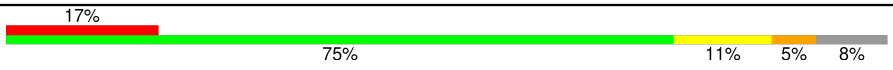
Mol	Chain	Length	Quality of chain
7	G	151	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15326 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 ACTIN-LIKE PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3212	2063	536	597	16	0	0	0

- Molecule 2 is a protein called ACTIN-LIKE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	190	1515	974	259	278	4	0	0	0

- Molecule 3 is a protein called ARP2/3 COMPLEX 41 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	354	2757	1747	487	504	19	0	0	0

- Molecule 4 is a protein called ARP2/3 COMPLEX 34 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	284	2291	1456	397	430	8	0	0	0

- Molecule 5 is a protein called ARP2/3 COMPLEX 21 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	174	1414	908	236	261	9	0	0	0

- Molecule 6 is a protein called ARP2/3 COMPLEX 20 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1369	875	239	246	9			

- Molecule 7 is a protein called ARP2/3 COMPLEX 16 KDA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	139	Total	C	N	O	S	0	0	0
			1058	661	185	209	3			

- Molecule 8 is water.

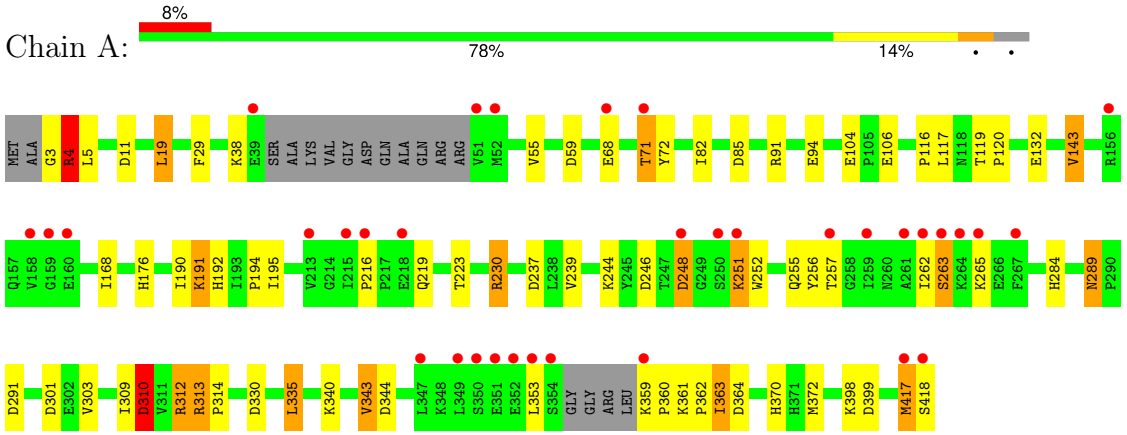
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	364	Total	O	27	0
			364	364		
8	B	209	Total	O	14	0
			209	209		
8	C	338	Total	O	30	0
			338	338		
8	D	355	Total	O	22	0
			355	355		
8	E	111	Total	O	12	0
			111	111		
8	F	230	Total	O	14	0
			230	230		
8	G	103	Total	O	9	0
			103	103		

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.

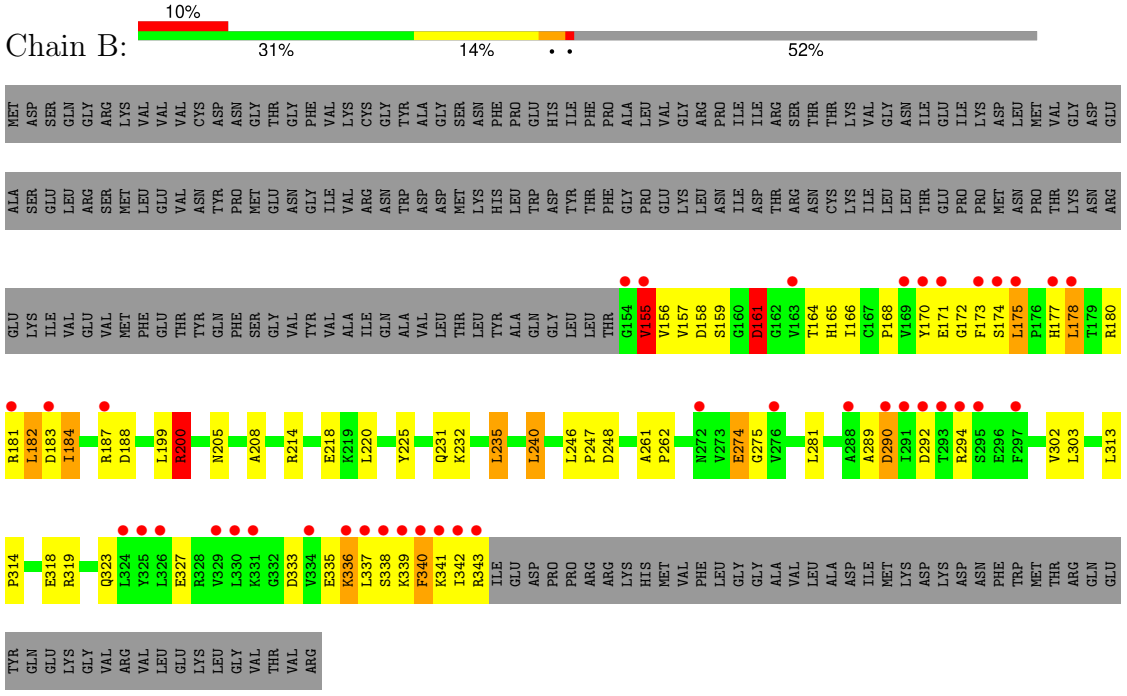
- Molecule 1: ACTIN-LIKE PROTEIN 3

Chain A:



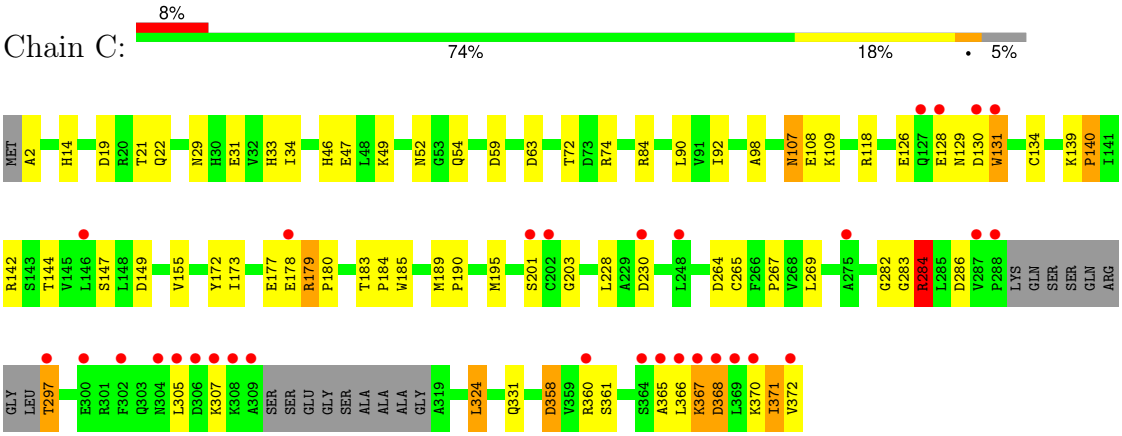
- Molecule 2: ACTIN-LIKE PROTEIN 2

Chain B:



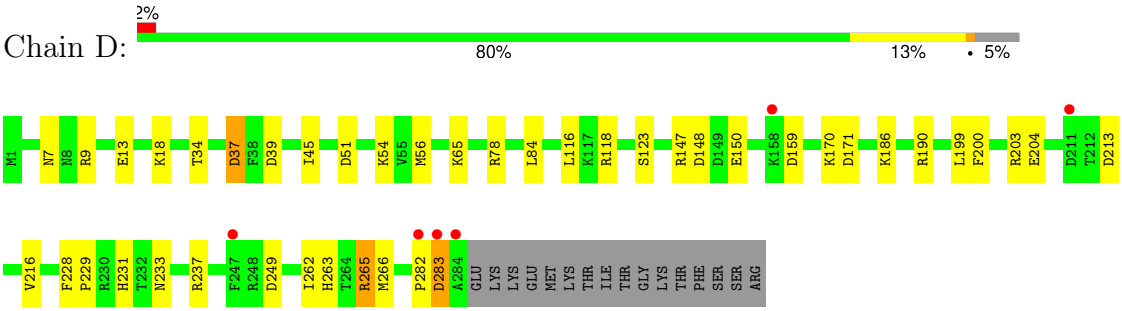
- Molecule 3: ARP2/3 COMPLEX 41 KDA SUBUNIT

Chain C:



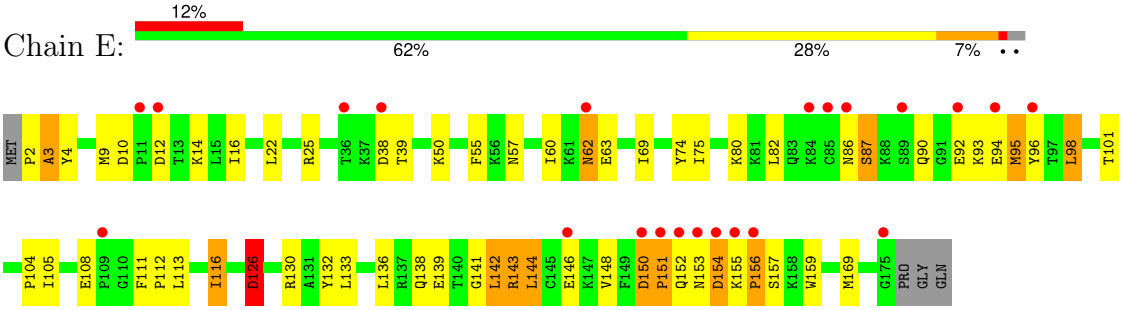
• Molecule 4: ARP2/3 COMPLEX 34 KDA SUBUNIT

Chain D:



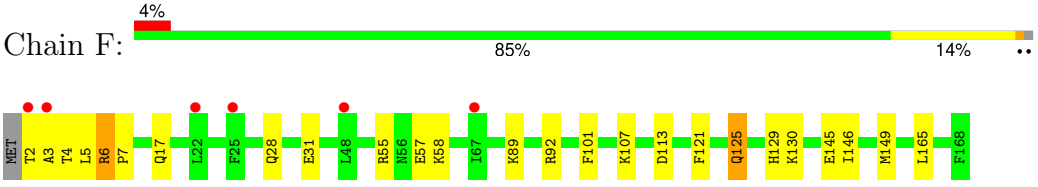
• Molecule 5: ARP2/3 COMPLEX 21 KDA SUBUNIT

Chain E:



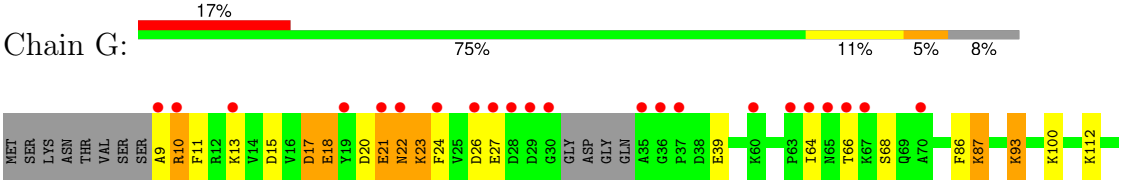
• Molecule 6: ARP2/3 COMPLEX 20 KDA SUBUNIT

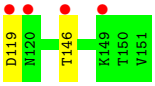
Chain F:



• Molecule 7: ARP2/3 COMPLEX 16 KDA SUBUNIT

Chain G:




D119
N120
T146
K149
T150
V151

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.71Å 130.40Å 204.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 41.54 – 2.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 92.1 (41.54-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.251 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.6	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	15326	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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	0.49	0/3293	0.79	13/4467 (0.3%)
2	B	0.40	0/1543	0.69	8/2084 (0.4%)
3	C	0.51	0/2826	0.79	6/3832 (0.2%)
4	D	0.53	0/2340	0.79	8/3160 (0.3%)
5	E	0.38	0/1448	0.70	5/1953 (0.3%)
6	F	0.56	0/1391	0.73	1/1867 (0.1%)
7	G	0.38	0/1070	0.73	3/1441 (0.2%)
All	All	0.48	0/13911	0.76	44/18804 (0.2%)

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	59	ASP	CB-CG-OD2	7.20	124.78	118.30
4	D	148	ASP	CB-CG-OD2	6.73	124.36	118.30
4	D	265	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	4	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	11	ASP	CB-CG-OD2	6.42	124.08	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3212	0	3163	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1515	0	1548	57	0
3	C	2757	0	2713	96	0
4	D	2291	0	2257	38	0
5	E	1414	0	1416	75	0
6	F	1369	0	1410	33	0
7	G	1058	0	1065	26	0
8	A	364	0	0	13	0
8	B	209	0	0	15	0
8	C	338	0	0	36	0
8	D	355	0	0	15	0
8	E	111	0	0	4	0
8	F	230	0	0	5	0
8	G	103	0	0	8	0
All	All	15326	0	13572	373	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.

The worst 5 of 373 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)
5:E:152:GLN:CB	5:E:155:LYS:NZ	1.85	1.38
2:B:165:HIS:CD2	2:B:181:ARG:HG2	1.58	1.37
5:E:152:GLN:HB3	5:E:155:LYS:CE	1.59	1.30
5:E:152:GLN:CB	5:E:155:LYS:CE	2.12	1.27
3:C:307:LYS:CE	8:C:568:HOH:O	1.63	1.26

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	395/418 (94%)	377 (95%)	16 (4%)	2 (0%)	29 23
2	B	188/394 (48%)	167 (89%)	15 (8%)	6 (3%)	4 1
3	C	348/372 (94%)	328 (94%)	18 (5%)	2 (1%)	25 19
4	D	282/300 (94%)	275 (98%)	6 (2%)	1 (0%)	34 30
5	E	172/178 (97%)	160 (93%)	8 (5%)	4 (2%)	6 2
6	F	165/168 (98%)	160 (97%)	5 (3%)	0	100 100
7	G	135/151 (89%)	130 (96%)	2 (2%)	3 (2%)	6 2
All	All	1685/1981 (85%)	1597 (95%)	70 (4%)	18 (1%)	14 8

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ARG
2	B	155	VAL
2	B	171	GLU
2	B	336	LYS
4	D	283	ASP

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	352/363 (97%)	335 (95%)	17 (5%)	25 22
2	B	165/345 (48%)	151 (92%)	14 (8%)	10 6
3	C	301/313 (96%)	289 (96%)	12 (4%)	31 29
4	D	249/264 (94%)	242 (97%)	7 (3%)	43 44
5	E	156/159 (98%)	141 (90%)	15 (10%)	8 5
6	F	154/155 (99%)	150 (97%)	4 (3%)	46 48
7	G	114/124 (92%)	104 (91%)	10 (9%)	10 6
All	All	1491/1723 (86%)	1412 (95%)	79 (5%)	22 18

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	98	LEU
7	G	27	GLU
5	E	116	ILE
6	F	6	ARG
7	G	86	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	65	ASN
7	G	96	GLN
3	C	331	GLN
6	F	154	ASN
3	C	303	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

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	401/418 (95%)	0.49	34 (8%) 10 10	18, 35, 76, 97	0
2	B	190/394 (48%)	0.93	39 (20%) 1 0	22, 46, 91, 109	0
3	C	354/372 (95%)	0.45	31 (8%) 10 9	20, 30, 76, 106	0
4	D	284/300 (94%)	0.20	6 (2%) 63 62	18, 30, 44, 55	0
5	E	174/178 (97%)	0.71	22 (12%) 3 3	33, 48, 77, 80	0
6	F	167/168 (99%)	0.18	6 (3%) 42 42	18, 26, 37, 58	0
7	G	139/151 (92%)	0.94	26 (18%) 1 1	23, 47, 95, 104	0
All	All	1709/1981 (86%)	0.51	164 (9%) 8 7	18, 34, 80, 109	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	284	ALA	14.3
7	G	35	ALA	9.0
3	C	309	ALA	8.8
5	E	96	TYR	8.3
3	C	308	LYS	7.8

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 monosaccharides 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.