wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 02:16 AM EDT

PDB ID	:	3FEY
Title	:	Crystal structure of the CBC-importin alpha complex.
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Deposited on	:	2008-12-01
Resolution	:	2.20 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 (i)) were used in the production of this report:

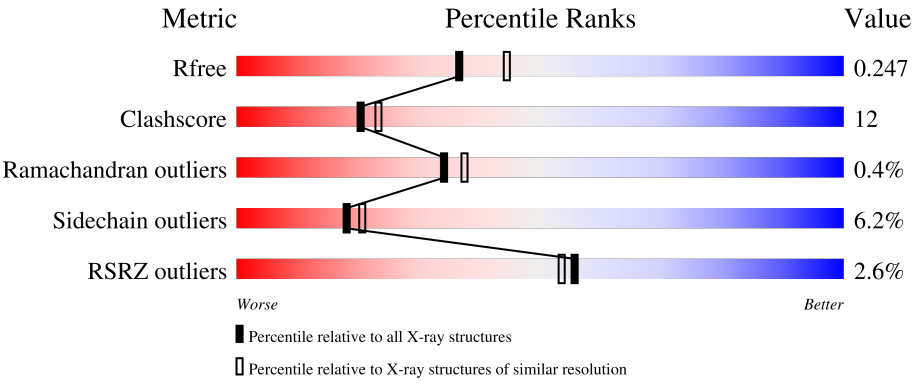
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	790	2% 74% 19%
2	B	156	5% 47% 12% 38%
3	C	467	2% 68% 22% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10746 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 Nuclear cap-binding protein subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	3	0
			6242	4007	1067	1130	38			

- Molecule 2 is a protein called Nuclear cap-binding protein subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			792	501	129	157	5			

- Molecule 3 is a protein called Importin subunit alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	428	Total	C	N	O	S	0	1	0
			3258	2074	547	626	11			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	MET	-	expression tag	UNP P52292
C	530	HIS	-	expression tag	UNP P52292
C	531	HIS	-	expression tag	UNP P52292
C	532	HIS	-	expression tag	UNP P52292
C	533	HIS	-	expression tag	UNP P52292
C	534	HIS	-	expression tag	UNP P52292
C	535	HIS	-	expression tag	UNP P52292

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	282	Total	O	0	0
			282	282		

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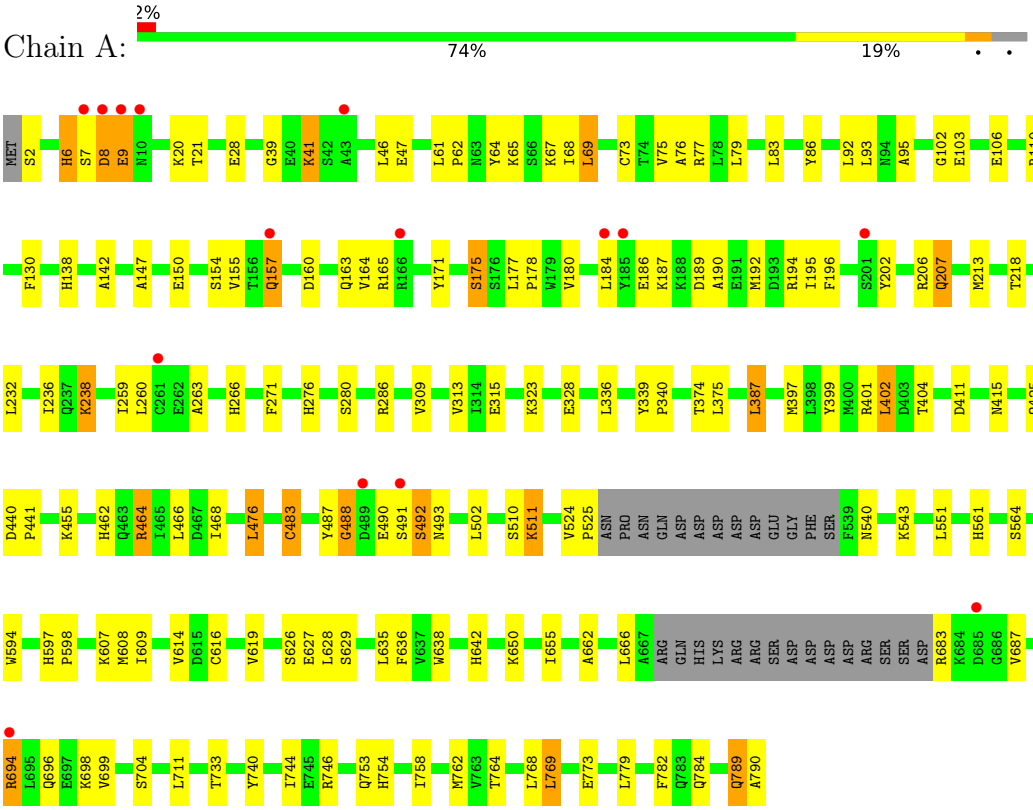
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	43	Total O 43 43	0	0
4	C	129	Total O 129 129	0	0

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.

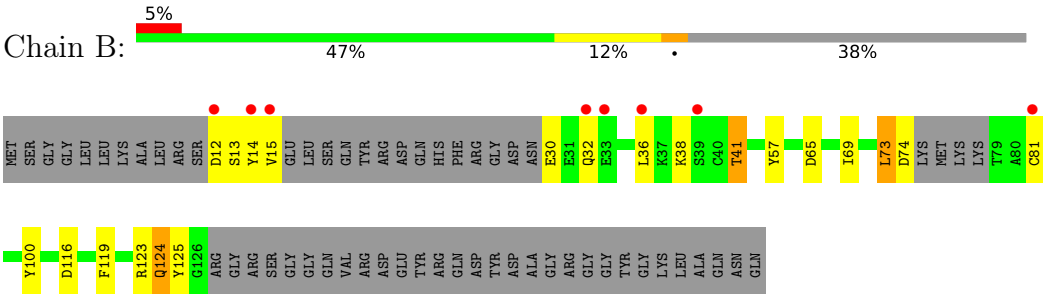
• Molecule 1: Nuclear cap-binding protein subunit 1

Chain A:



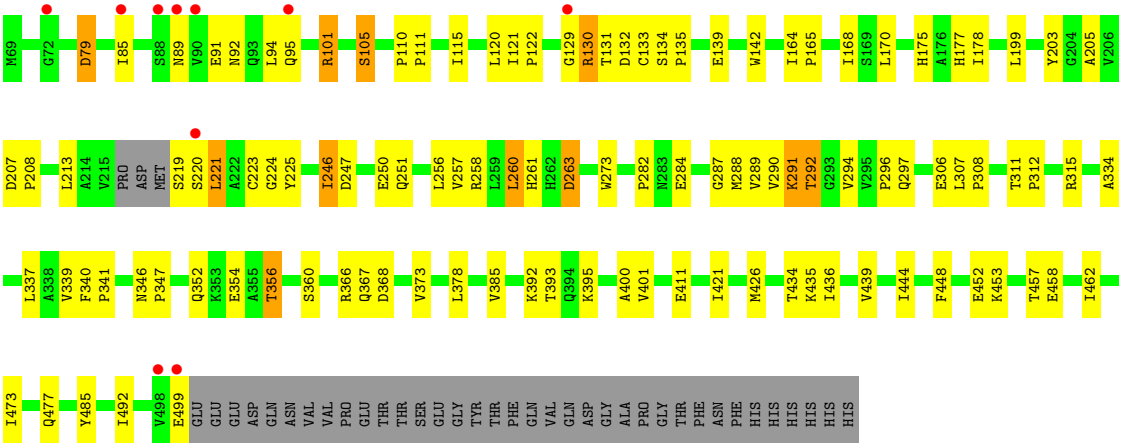
• Molecule 2: Nuclear cap-binding protein subunit 2

Chain B:



• Molecule 3: Importin subunit alpha-2

Chain C:


M69 G72 D79 I85 S88 N89 V90 E91 N92 Q93 L94 Q95 R101 S105 P110 P111 I115 L120 I121 P122 G129 R130 T131 D132 C133 S134 P135 E139 W142 I164 P165 I168 S169 L170 H175 A176 H177 I178 L199 Y203 G204 A205 V206
D207 P208 L213 A214 V215 PRO ASP MET S219 S220 L221 A222 C223 G224 Y225 I246 D247 E250 Q251 L256 V257 R258 L259 L260 H261 H262 D263 W273 P282 N283 E284 G287 M288 V289 V290 K291 T292 G293 V294 V296 P296 Q297 E306 L307 P308 T311 P312 R315 A334
L337 A338 V339 F340 P341 N346 P347 Q352 K353 E354 A355 T356 S360 R366 Q367 D368 V373 L378 V385 K392 T393 Q394 K395 A400 V401 E411 I421 M426 T434 K435 I436 V439 I444 F448 E452 K453 T457 E458 I462
I473 Q477 Y485 I492 V498 E499 GLU GLU GLU ASP GLN ASN VAL VAL PRO GLU THR THR SER GLU GLY TYR THR PHE GLN VAL GLN ASP GLY ALA PRO GLY THR PHE ASN PHE HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.84Å 104.50Å 108.56Å 90.00° 109.04° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 14.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.20) 97.2 (14.98-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.192 , 0.238 0.203 , 0.247	Depositor DCC
R_{free} test set	4376 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.2	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	0.95	EDS
Total number of atoms	10746	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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	0.52	2/6407 (0.0%)	0.61	0/8685
2	B	0.60	1/804 (0.1%)	0.66	0/1075
3	C	0.53	0/3317	0.61	0/4525
All	All	0.53	3/10528 (0.0%)	0.62	0/14285

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	483	CYS	CB-SG	-6.32	1.71	1.82
1	A	616	CYS	CB-SG	5.18	1.91	1.82
2	B	81	CYS	CB-SG	-5.07	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	ASP	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	6242	0	6221	136	0
2	B	792	0	756	20	0
3	C	3258	0	3323	108	0
4	A	282	0	0	12	0
4	B	43	0	0	4	0
4	C	129	0	0	13	0
All	All	10746	0	10300	255	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 12.

The worst 5 of 255 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)
3:C:246:ILE:CD1	3:C:246:ILE:H	1.55	1.15
1:A:6[A]:HIS:NE2	3:C:354:GLU:OE2	1.83	1.11
3:C:219:SER:HB2	3:C:220:SER:CA	1.80	1.10
3:C:246:ILE:HD13	3:C:246:ILE:N	1.67	1.07
3:C:219:SER:CB	3:C:220:SER:HA	1.73	1.05

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	758/790 (96%)	740 (98%)	14 (2%)	4 (0%)	29 31
2	B	91/156 (58%)	91 (100%)	0	0	100 100
3	C	425/467 (91%)	416 (98%)	8 (2%)	1 (0%)	47 55
All	All	1274/1413 (90%)	1247 (98%)	22 (2%)	5 (0%)	34 37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	SER
3	C	130	ARG
1	A	488	GLY
1	A	9	GLU
1	A	511	LYS

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	699/724 (96%)	652 (93%)	47 (7%)	16	18
2	B	84/130 (65%)	77 (92%)	7 (8%)	11	11
3	C	362/396 (91%)	344 (95%)	18 (5%)	24	30
All	All	1145/1250 (92%)	1073 (94%)	72 (6%)	18	20

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	221	LEU
3	C	457	THR
3	C	246	ILE
3	C	292	THR
1	A	464	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	HIS
3	C	137	GLN
3	C	261	HIS
1	A	138	HIS
1	A	49	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

There are no monosaccharides 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	761/790 (96%)	-0.21	15 (1%)	65	63	9, 23, 30, 44	41 (5%)
2	B	97/156 (62%)	0.28	8 (8%)	11	10	11, 17, 93, 111	5 (5%)
3	C	428/467 (91%)	-0.21	10 (2%)	60	58	10, 20, 35, 42	25 (5%)
All	All	1286/1413 (91%)	-0.17	33 (2%)	56	53	9, 22, 33, 111	71 (5%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	VAL	7.7
1	A	491	SER	6.6
2	B	14	TYR	6.3
2	B	39	SER	5.8
1	A	8	ASP	5.7

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 (i)

There are no such residues in this entry.