wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:19 AM GMT

PDB ID	:	3E5Q
Title	:	Unbound Oxidised CprK
Authors	:	Levy, C.
Deposited on	:	2008-08-14
Resolution	:	3.20 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
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:

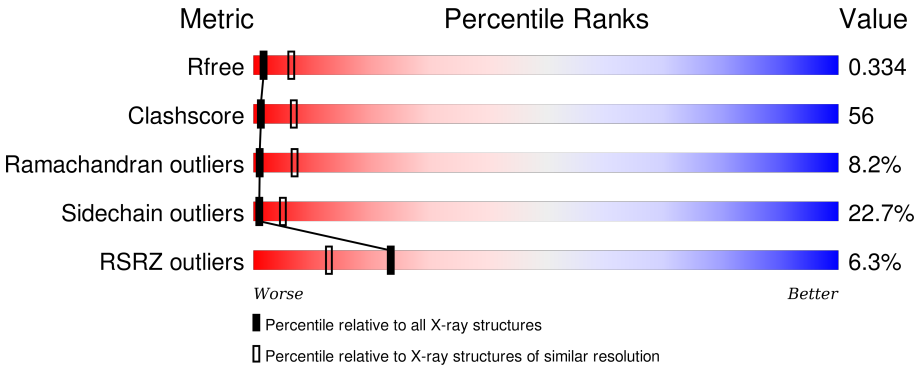
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	250	6% 23% 39% 17% • 19%
1	B	250	2% 20% 38% 20% • 20%
1	C	250	9% 24% 42% 15% • 19%
1	D	250	8% 20% 43% 16% • 20%
1	E	250	4% 20% 46% 13% • 19%

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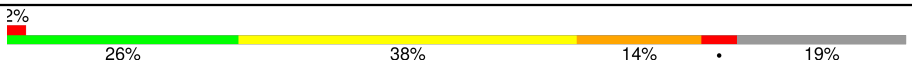
Mol	Chain	Length	Quality of chain
1	F	250	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9641 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 Cyclic nucleotide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1600	1034	265	293	8			
1	B	201	Total	C	N	O	S	0	0	0
			1611	1043	268	292	8			
1	C	203	Total	C	N	O	S	0	0	0
			1605	1037	266	294	8			
1	D	201	Total	C	N	O	S	0	0	0
			1605	1040	265	292	8			
1	E	203	Total	C	N	O	S	0	0	0
			1605	1037	266	294	8			
1	F	203	Total	C	N	O	S	0	0	0
			1615	1045	269	293	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	SER	-	EXPRESSION TAG	UNP Q18R04
A	234	ASP	-	EXPRESSION TAG	UNP Q18R04
A	235	PRO	-	EXPRESSION TAG	UNP Q18R04
A	236	ASN	-	EXPRESSION TAG	UNP Q18R04
A	237	SER	-	EXPRESSION TAG	UNP Q18R04
A	238	SER	-	EXPRESSION TAG	UNP Q18R04
A	239	SER	-	EXPRESSION TAG	UNP Q18R04
A	240	VAL	-	EXPRESSION TAG	UNP Q18R04
A	241	ASP	-	EXPRESSION TAG	UNP Q18R04
A	242	LYS	-	EXPRESSION TAG	UNP Q18R04
A	243	LEU	-	EXPRESSION TAG	UNP Q18R04
A	244	ALA	-	EXPRESSION TAG	UNP Q18R04
A	245	ALA	-	EXPRESSION TAG	UNP Q18R04
A	246	ALA	-	EXPRESSION TAG	UNP Q18R04
A	247	LEU	-	EXPRESSION TAG	UNP Q18R04
A	248	ASP	-	EXPRESSION TAG	UNP Q18R04
A	249	HIS	-	EXPRESSION TAG	UNP Q18R04

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Chain	Residue	Modelled	Actual	Comment	Reference
A	250	HIS	-	EXPRESSION TAG	UNP Q18R04
B	233	SER	-	EXPRESSION TAG	UNP Q18R04
B	234	ASP	-	EXPRESSION TAG	UNP Q18R04
B	235	PRO	-	EXPRESSION TAG	UNP Q18R04
B	236	ASN	-	EXPRESSION TAG	UNP Q18R04
B	237	SER	-	EXPRESSION TAG	UNP Q18R04
B	238	SER	-	EXPRESSION TAG	UNP Q18R04
B	239	SER	-	EXPRESSION TAG	UNP Q18R04
B	240	VAL	-	EXPRESSION TAG	UNP Q18R04
B	241	ASP	-	EXPRESSION TAG	UNP Q18R04
B	242	LYS	-	EXPRESSION TAG	UNP Q18R04
B	243	LEU	-	EXPRESSION TAG	UNP Q18R04
B	244	ALA	-	EXPRESSION TAG	UNP Q18R04
B	245	ALA	-	EXPRESSION TAG	UNP Q18R04
B	246	ALA	-	EXPRESSION TAG	UNP Q18R04
B	247	LEU	-	EXPRESSION TAG	UNP Q18R04
B	248	ASP	-	EXPRESSION TAG	UNP Q18R04
B	249	HIS	-	EXPRESSION TAG	UNP Q18R04
B	250	HIS	-	EXPRESSION TAG	UNP Q18R04
C	233	SER	-	EXPRESSION TAG	UNP Q18R04
C	234	ASP	-	EXPRESSION TAG	UNP Q18R04
C	235	PRO	-	EXPRESSION TAG	UNP Q18R04
C	236	ASN	-	EXPRESSION TAG	UNP Q18R04
C	237	SER	-	EXPRESSION TAG	UNP Q18R04
C	238	SER	-	EXPRESSION TAG	UNP Q18R04
C	239	SER	-	EXPRESSION TAG	UNP Q18R04
C	240	VAL	-	EXPRESSION TAG	UNP Q18R04
C	241	ASP	-	EXPRESSION TAG	UNP Q18R04
C	242	LYS	-	EXPRESSION TAG	UNP Q18R04
C	243	LEU	-	EXPRESSION TAG	UNP Q18R04
C	244	ALA	-	EXPRESSION TAG	UNP Q18R04
C	245	ALA	-	EXPRESSION TAG	UNP Q18R04
C	246	ALA	-	EXPRESSION TAG	UNP Q18R04
C	247	LEU	-	EXPRESSION TAG	UNP Q18R04
C	248	ASP	-	EXPRESSION TAG	UNP Q18R04
C	249	HIS	-	EXPRESSION TAG	UNP Q18R04
C	250	HIS	-	EXPRESSION TAG	UNP Q18R04
D	233	SER	-	EXPRESSION TAG	UNP Q18R04
D	234	ASP	-	EXPRESSION TAG	UNP Q18R04
D	235	PRO	-	EXPRESSION TAG	UNP Q18R04
D	236	ASN	-	EXPRESSION TAG	UNP Q18R04
D	237	SER	-	EXPRESSION TAG	UNP Q18R04

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Chain	Residue	Modelled	Actual	Comment	Reference
D	238	SER	-	EXPRESSION TAG	UNP Q18R04
D	239	SER	-	EXPRESSION TAG	UNP Q18R04
D	240	VAL	-	EXPRESSION TAG	UNP Q18R04
D	241	ASP	-	EXPRESSION TAG	UNP Q18R04
D	242	LYS	-	EXPRESSION TAG	UNP Q18R04
D	243	LEU	-	EXPRESSION TAG	UNP Q18R04
D	244	ALA	-	EXPRESSION TAG	UNP Q18R04
D	245	ALA	-	EXPRESSION TAG	UNP Q18R04
D	246	ALA	-	EXPRESSION TAG	UNP Q18R04
D	247	LEU	-	EXPRESSION TAG	UNP Q18R04
D	248	ASP	-	EXPRESSION TAG	UNP Q18R04
D	249	HIS	-	EXPRESSION TAG	UNP Q18R04
D	250	HIS	-	EXPRESSION TAG	UNP Q18R04
E	233	SER	-	EXPRESSION TAG	UNP Q18R04
E	234	ASP	-	EXPRESSION TAG	UNP Q18R04
E	235	PRO	-	EXPRESSION TAG	UNP Q18R04
E	236	ASN	-	EXPRESSION TAG	UNP Q18R04
E	237	SER	-	EXPRESSION TAG	UNP Q18R04
E	238	SER	-	EXPRESSION TAG	UNP Q18R04
E	239	SER	-	EXPRESSION TAG	UNP Q18R04
E	240	VAL	-	EXPRESSION TAG	UNP Q18R04
E	241	ASP	-	EXPRESSION TAG	UNP Q18R04
E	242	LYS	-	EXPRESSION TAG	UNP Q18R04
E	243	LEU	-	EXPRESSION TAG	UNP Q18R04
E	244	ALA	-	EXPRESSION TAG	UNP Q18R04
E	245	ALA	-	EXPRESSION TAG	UNP Q18R04
E	246	ALA	-	EXPRESSION TAG	UNP Q18R04
E	247	LEU	-	EXPRESSION TAG	UNP Q18R04
E	248	ASP	-	EXPRESSION TAG	UNP Q18R04
E	249	HIS	-	EXPRESSION TAG	UNP Q18R04
E	250	HIS	-	EXPRESSION TAG	UNP Q18R04
F	233	SER	-	EXPRESSION TAG	UNP Q18R04
F	234	ASP	-	EXPRESSION TAG	UNP Q18R04
F	235	PRO	-	EXPRESSION TAG	UNP Q18R04
F	236	ASN	-	EXPRESSION TAG	UNP Q18R04
F	237	SER	-	EXPRESSION TAG	UNP Q18R04
F	238	SER	-	EXPRESSION TAG	UNP Q18R04
F	239	SER	-	EXPRESSION TAG	UNP Q18R04
F	240	VAL	-	EXPRESSION TAG	UNP Q18R04
F	241	ASP	-	EXPRESSION TAG	UNP Q18R04
F	242	LYS	-	EXPRESSION TAG	UNP Q18R04
F	243	LEU	-	EXPRESSION TAG	UNP Q18R04

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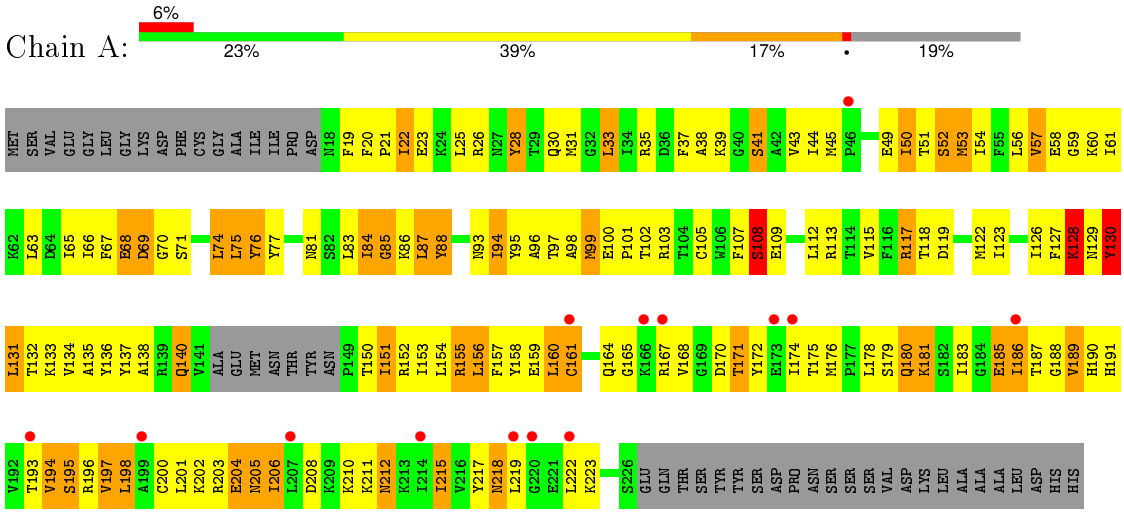
Chain	Residue	Modelled	Actual	Comment	Reference
F	244	ALA	-	EXPRESSION TAG	UNP Q18R04
F	245	ALA	-	EXPRESSION TAG	UNP Q18R04
F	246	ALA	-	EXPRESSION TAG	UNP Q18R04
F	247	LEU	-	EXPRESSION TAG	UNP Q18R04
F	248	ASP	-	EXPRESSION TAG	UNP Q18R04
F	249	HIS	-	EXPRESSION TAG	UNP Q18R04
F	250	HIS	-	EXPRESSION TAG	UNP Q18R04

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.

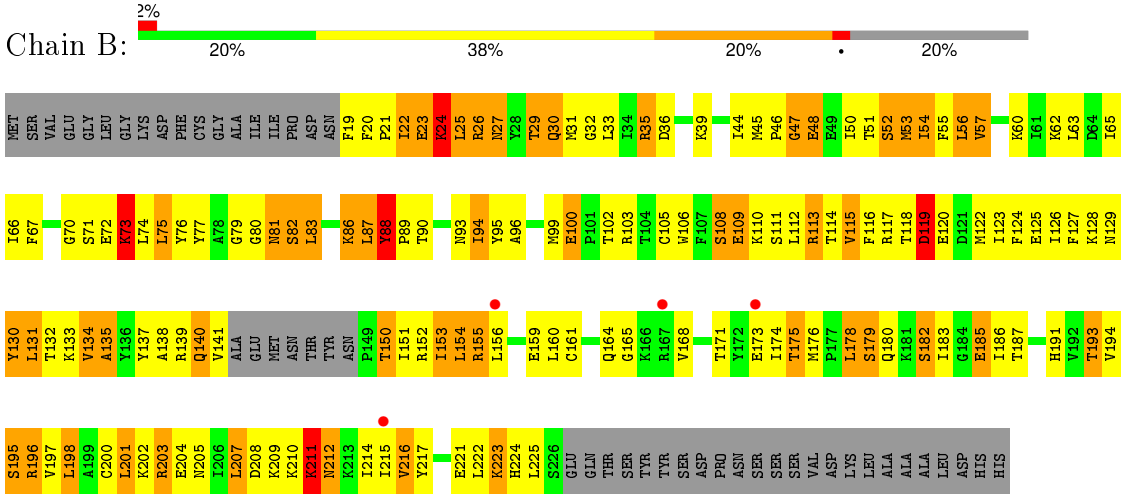
- Molecule 1: Cyclic nucleotide-binding protein

Chain A:



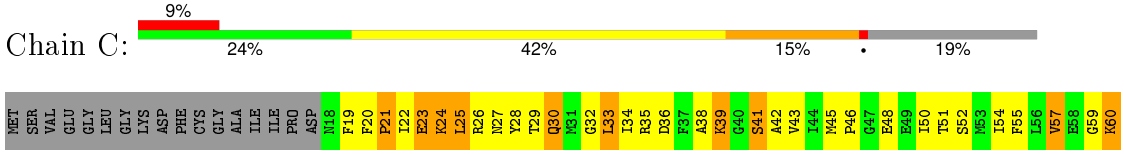
- Molecule 1: Cyclic nucleotide-binding protein

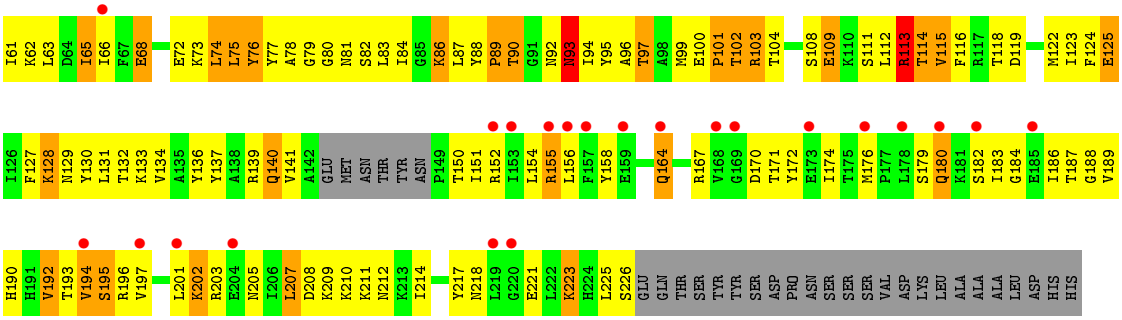
Chain B:



- Molecule 1: Cyclic nucleotide-binding protein

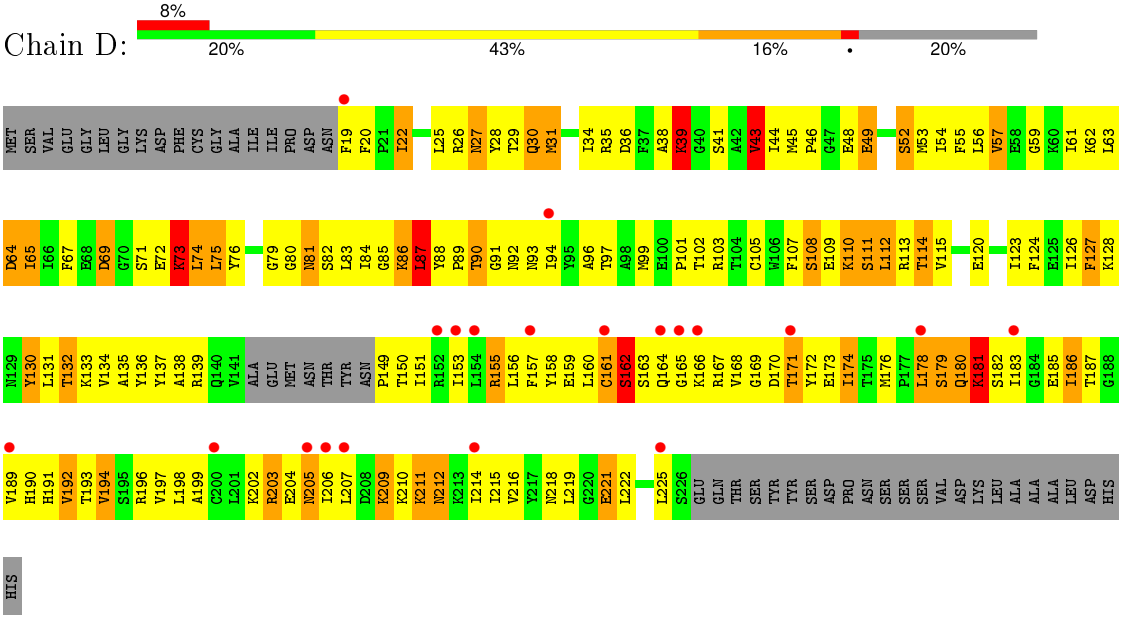
Chain C:





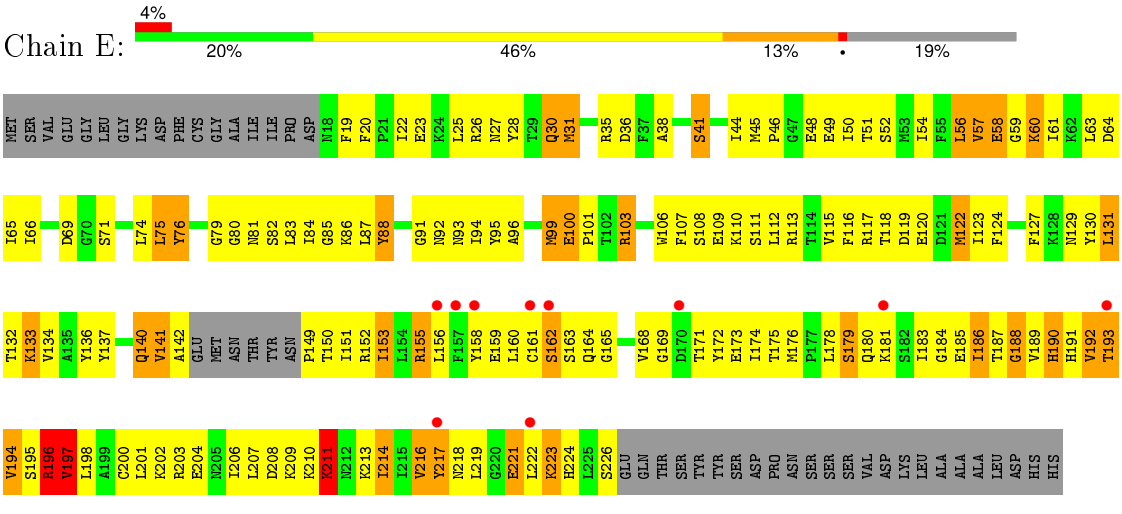
• Molecule 1: Cyclic nucleotide-binding protein

Chain D:



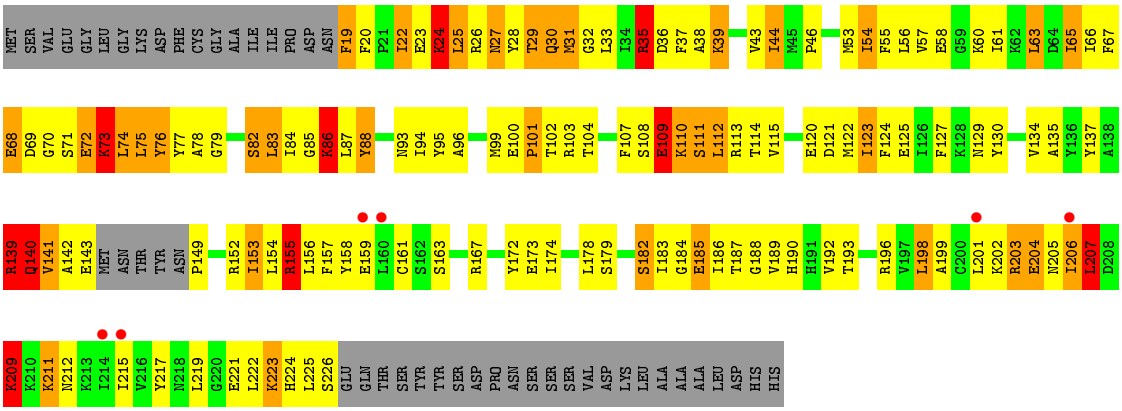
• Molecule 1: Cyclic nucleotide-binding protein

Chain E:



• Molecule 1: Cyclic nucleotide-binding protein

Chain F:


MET SER VAL GLU GLY LEU GLY LYS ASP PHE CYS GLY ALA ILE ILE PRO ASP ASN F19 F20 P21 I22 E23 K24 L25 R26 N27 Y28 T29 Q30 M31 G32 L33 I34 R35 D36 F37 A38 K39 V43 I44 M45 P46 M53 I54 F55 L56 V57 E58 G59 K60 I61 K62 L63 D64 I65 I66 F67
E68 D69 G70 S71 E72 K73 L74 L75 Y76 Y77 A78 G79 S82 L83 I84 G85 K86 L87 Y88 N93 I94 Y95 A96 M99 E100 P101 T102 R103 T104 F107 S108 E109 K110 S111 L112 R113 T114 V115 E120 D121 M122 I123 F124 E125 I126 F127 K128 N129 Y130 V134 A135 Y136 Y137 A138
R139 Q140 V141 A142 E143 MET ASN THR TYR ASN P149 R152 I153 L154 R155 L156 F157 Y158 E159 L160 C161 S162 S163 R167 Y172 E173 I174 L178 S179 S182 I183 G184 E185 I186 T187 G188 V189 H190 H191 V192 T193 R196 V197 L198 A199 C200 L201 K202 R203 E204 N205 I206 L207 D208
K209 K210 K211 N212 K213 I214 I215 V216 Y217 N218 L219 G220 E221 L222 K223 H224 L225 S226 GLU GLN THR SER TYR TYR SER ASP PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA LEU ASP 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	79.41Å 64.71Å 148.35Å 90.00° 105.29° 90.00°	Depositor
Resolution (Å)	142.86 – 3.20 46.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	79.8 (142.86-3.20) 70.4 (46.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.258 , 0.318 0.329 , 0.334	Depositor DCC
R_{free} test set	1711 reflections (10.01%)	DCC
Wilson B-factor (Å^2)	72.2	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.0	EDS
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	3 of 17150 reflections (0.017%)	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	9641	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.15	4/1630 (0.2%)	1.19	5/2200 (0.2%)
1	B	1.17	5/1641 (0.3%)	1.26	12/2209 (0.5%)
1	C	1.02	1/1635 (0.1%)	1.09	0/2207
1	D	0.92	1/1635 (0.1%)	1.01	2/2202 (0.1%)
1	E	0.98	0/1635	1.11	6/2207 (0.3%)
1	F	0.97	2/1645 (0.1%)	1.08	8/2215 (0.4%)
All	All	1.04	13/9821 (0.1%)	1.13	33/13240 (0.2%)

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
1	B	0	3
1	D	0	2
1	E	0	2
1	F	0	1
All	All	0	9

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	CYS	CB-SG	7.62	1.95	1.82
1	A	130	TYR	CE2-CZ	6.38	1.46	1.38
1	A	130	TYR	CG-CD1	6.17	1.47	1.39
1	C	23	GLU	CG-CD	6.17	1.61	1.51
1	B	109	GLU	CG-CD	5.92	1.60	1.51

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	26	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	E	83	LEU	CA-CB-CG	-8.52	95.70	115.30
1	B	119	ASP	CB-CG-OD1	-8.05	111.06	118.30
1	F	207	LEU	CA-CB-CG	7.33	132.15	115.30
1	B	130	TYR	CA-CB-CG	-7.25	99.62	113.40

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	THR	Peptide
1	B	47	GLY	Peptide
1	B	71	SER	Peptide
1	B	88	TYR	Peptide
1	D	87	LEU	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	1600	0	1601	200	0
1	B	1611	0	1643	226	0
1	C	1605	0	1606	195	0
1	D	1605	0	1632	206	1
1	E	1605	0	1606	200	0
1	F	1615	0	1637	190	1
All	All	9641	0	9725	1081	1

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 56.

The worst 5 of 1081 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:35:ARG:NH1	1:A:37:PHE:HZ	1.42	1.14
1:D:44:ILE:HG21	1:D:94:ILE:HG22	1.32	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:LYS:HD3	1:E:99:MET:HE3	1.10	1.10
1:C:50:ILE:HB	1:C:86:LYS:HE2	1.26	1.09
1:B:22:ILE:HG13	1:B:22:ILE:O	1.48	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:NH1	1:F:35:ARG:NH1[1_656]	2.10	0.10

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	198/250 (79%)	140 (71%)	41 (21%)	17 (9%)	1 6
1	B	197/250 (79%)	146 (74%)	31 (16%)	20 (10%)	1 4
1	C	199/250 (80%)	151 (76%)	36 (18%)	12 (6%)	2 16
1	D	197/250 (79%)	144 (73%)	31 (16%)	22 (11%)	0 3
1	E	199/250 (80%)	152 (76%)	34 (17%)	13 (6%)	1 13
1	F	199/250 (80%)	156 (78%)	29 (15%)	14 (7%)	1 10
All	All	1189/1500 (79%)	889 (75%)	202 (17%)	98 (8%)	1 7

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ILE
1	A	205	ASN
1	A	206	ILE
1	A	212	ASN
1	A	218	ASN

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	170/220 (77%)	131 (77%)	39 (23%)	1	4
1	B	174/220 (79%)	133 (76%)	41 (24%)	1	4
1	C	170/220 (77%)	130 (76%)	40 (24%)	1	4
1	D	173/220 (79%)	134 (78%)	39 (22%)	1	5
1	E	170/220 (77%)	137 (81%)	33 (19%)	2	9
1	F	172/220 (78%)	130 (76%)	42 (24%)	1	3
All	All	1029/1320 (78%)	795 (77%)	234 (23%)	1	5

5 of 234 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	128	LYS
1	D	64	ASP
1	F	153	ILE
1	C	164	GLN
1	C	223	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	212	ASN
1	D	180	GLN
1	F	191	HIS
1	D	27	ASN
1	D	190	HIS

5.3.3 RNA (i)

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	202/250 (80%)	0.39	14 (6%) 20 11	74, 81, 85, 90	0
1	B	201/250 (80%)	0.30	4 (1%) 68 54	74, 79, 84, 87	0
1	C	203/250 (81%)	0.62	22 (10%) 8 4	73, 80, 85, 91	0
1	D	201/250 (80%)	0.47	20 (9%) 9 5	73, 80, 85, 89	0
1	E	203/250 (81%)	0.26	10 (4%) 33 20	75, 80, 84, 90	0
1	F	203/250 (81%)	0.23	6 (2%) 54 39	75, 80, 84, 87	0
All	All	1213/1500 (80%)	0.38	76 (6%) 23 13	73, 80, 85, 91	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	8.0
1	C	153	ILE	7.4
1	D	161	CYS	6.2
1	E	161	CYS	6.1
1	C	201	LEU	5.2

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 (i)

There are no such residues in this entry.