



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:16 PM 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 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/ValidationPDFNotes.html>

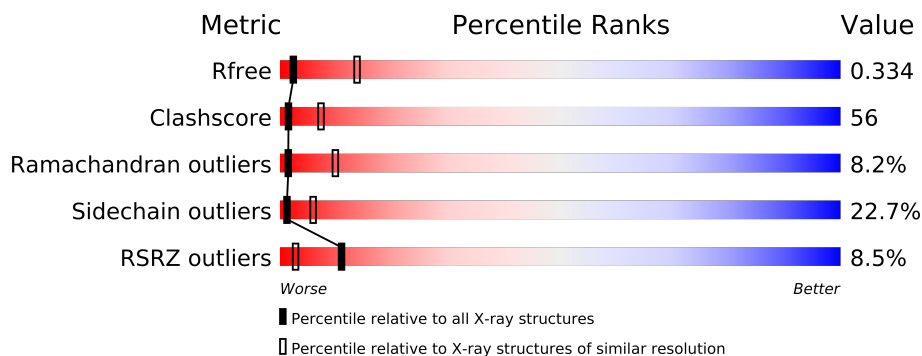
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	250	
1	B	250	
1	C	250	
1	D	250	
1	E	250	
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 hydrogen and 0 are deuterium.

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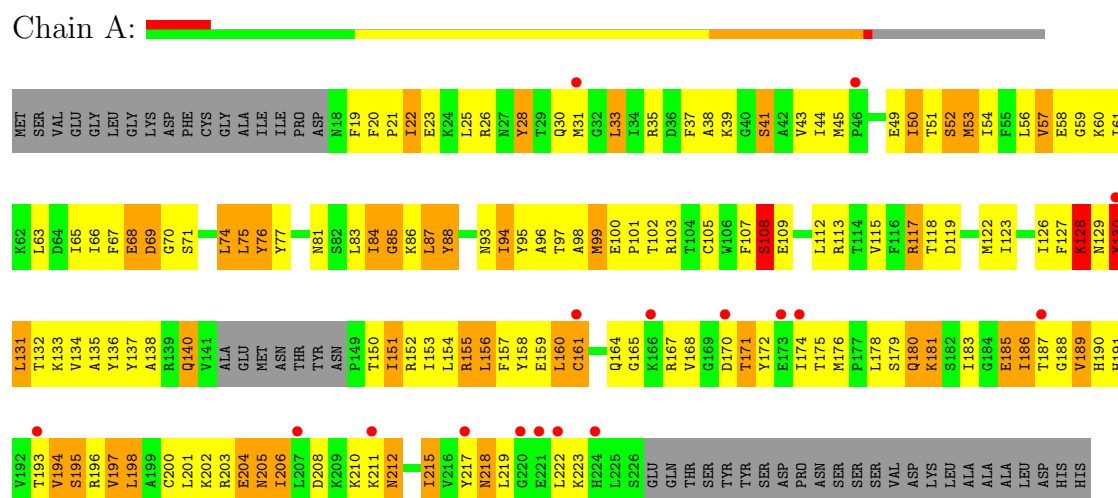
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Chain	Residue	Modelled	Actual	Comment	Reference
F	244	ALA	-	EXPRESSION TAG	UNP Q18R04
F	245	ALA	-	EXPRESSION TAG	UNP Q18R04
F	246	ALA	-	EXPRESSION TAG	UNP Q18R04
F	247	LEU	-	EXPRESSION TAG	UNP Q18R04
F	248	ASP	-	EXPRESSION TAG	UNP Q18R04
F	249	HIS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

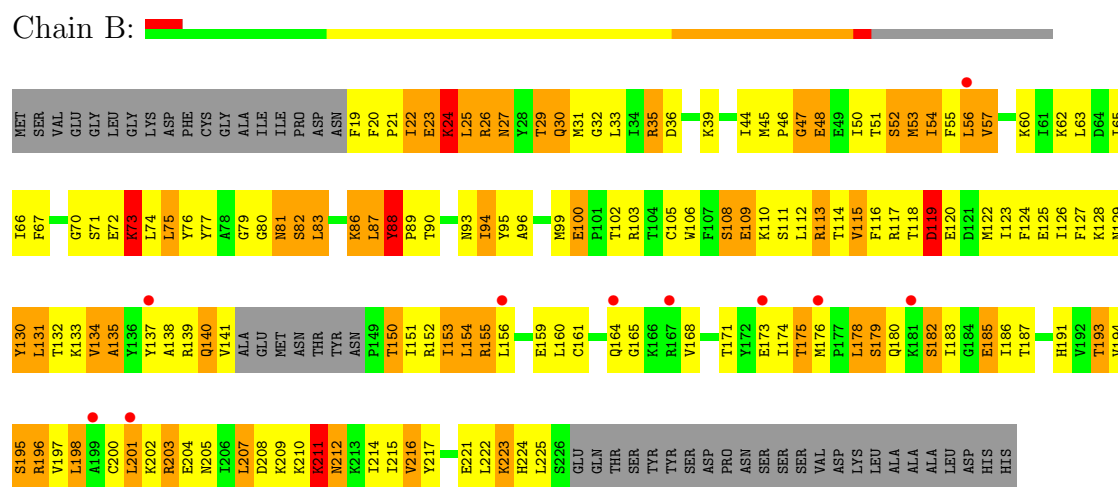
3 Residue-property plots

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.

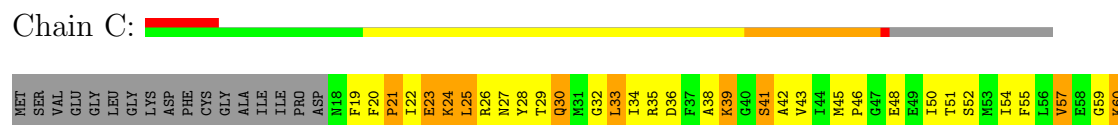
• Molecule 1: Cyclic nucleotide-binding protein

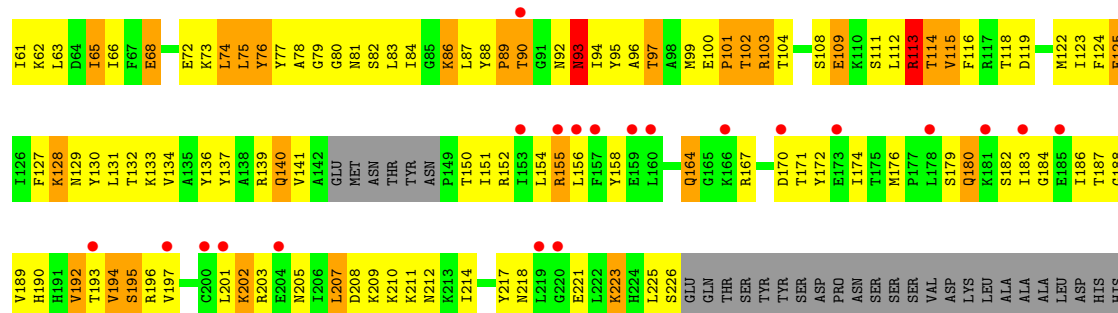


• Molecule 1: Cyclic nucleotide-binding protein



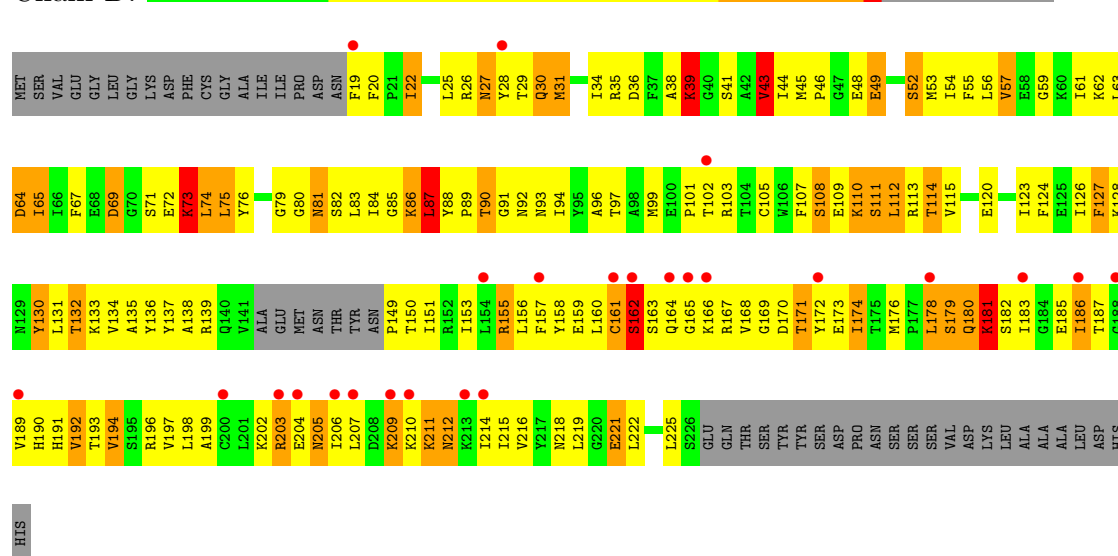
• Molecule 1: Cyclic nucleotide-binding protein





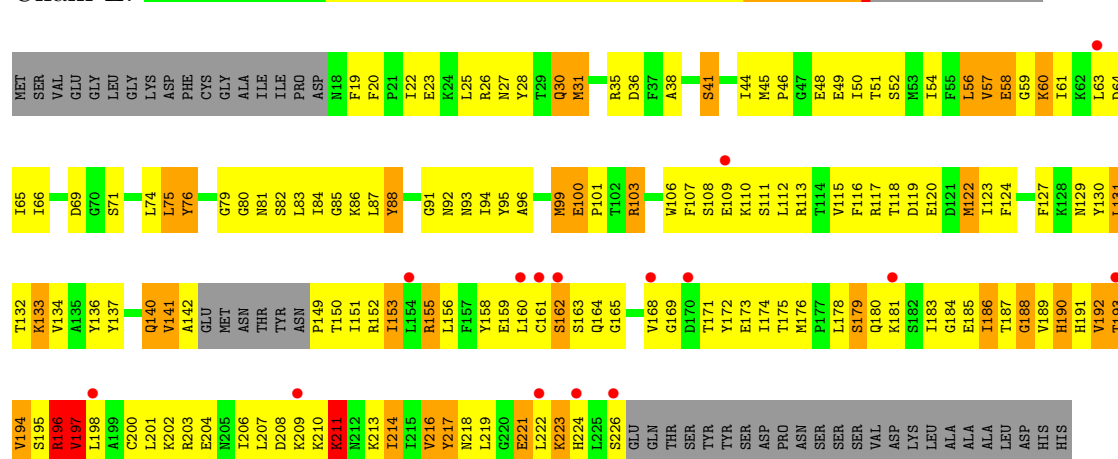
• Molecule 1: Cyclic nucleotide-binding protein

Chain D:



• Molecule 1: Cyclic nucleotide-binding protein

Chain E:



• Molecule 1: Cyclic nucleotide-binding protein

Chain F:

N205	A138	E68	MET
I206	R139	D69	SER
L207	Q140	G70	VAL
D208	V141	S71	GLY
K209	A142	E72	GLY
K210	E143	K73	LEU
K211	MET	L74	GLY
N212	ASN	L75	LYS
K213	THR	Y76	ASP
I214	TYR	Y77	PHE
I215	ASN	A78	CYS
V216	P149	G79	GLY
Y217			ALA
N218	R152	S82	ILE
L219	I153	L83	ILE
G220	L154	I84	PRO
E221	R155	G85	ASP
L222	L156	K86	ASN
K223	F157	L87	F19
H224	Y158	Y88	F20
L225	E159		P21
S226	L160	N93	I22
GLU	C161	I94	E23
GLN	S162	Y95	K24
THR	S163	A96	L25
SER			R26
TYR	R167	N99	N27
SER	V168	E100	Y28
ASP	G169	P101	T29
PRO		T102	Q30
ASN	Y172	R103	N31
SER	E173	T104	Q32
SER	I174	C105	L33
VAL	P177	W106	I34
ASP	L178	F107	R35
LYS	S179	S108	D36
LEU		K110	F37
ALA	S182	S111	A38
ALA	I183	L112	R39
ALA	G184	R113	V43
LEU	E185	T114	I44
ASP	I186	V115	N45
HIS	T187		P46
HIS	G188	E120	
	V189	D121	M53
	H190	M122	I54
	H191	I123	F55
	V192	F124	L56
	T193	E125	V57
		I126	E58
	R196	F127	G59
	V197	K128	K60
	L198	N129	I61
	A199	Y130	K62
	C200		L63
	L201	V134	D64
	K202	A136	I65
	R203	Y136	I66
	E204	Y137	P67

4 Data and refinement statistics

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) 69.6 (46.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	1710 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	EDS
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 17150 reflections (0.017%)	Xtriage
F_o, F_c correlation	0.79	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 56.

The worst 5 of 1081 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:E:60:LYS:HD3	1:E:99:MET:HE3	1.10	1.10

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

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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 ⓘ

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	5
1	B	174/220 (79%)	133 (76%)	41 (24%)	1	4
1	C	170/220 (77%)	130 (76%)	40 (24%)	1	5
1	D	173/220 (79%)	134 (78%)	39 (22%)	1	6
1	E	170/220 (77%)	137 (81%)	33 (19%)	2	10
1	F	172/220 (78%)	130 (76%)	42 (24%)	1	3
All	All	1029/1320 (78%)	795 (77%)	234 (23%)	1	6

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 ⓘ

There are no RNA chains 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, 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	202/250 (80%)	0.74	17 (8%) 11 3	74, 81, 85, 90	0
1	B	201/250 (80%)	0.62	10 (4%) 28 5	74, 79, 84, 87	0
1	C	203/250 (81%)	0.91	21 (10%) 7 2	73, 80, 85, 91	0
1	D	201/250 (80%)	0.82	25 (12%) 5 1	73, 80, 85, 89	0
1	E	203/250 (81%)	0.67	15 (7%) 14 3	75, 80, 84, 90	0
1	F	203/250 (81%)	0.69	15 (7%) 14 3	75, 80, 84, 87	0
All	All	1213/1500 (80%)	0.74	103 (8%) 11 3	73, 80, 85, 91	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	161	CYS	9.7
1	C	156	LEU	8.7
1	C	153	ILE	7.0
1	A	207	LEU	7.0
1	A	161	CYS	5.8

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 carbohydrates 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.