



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 06:40 am BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

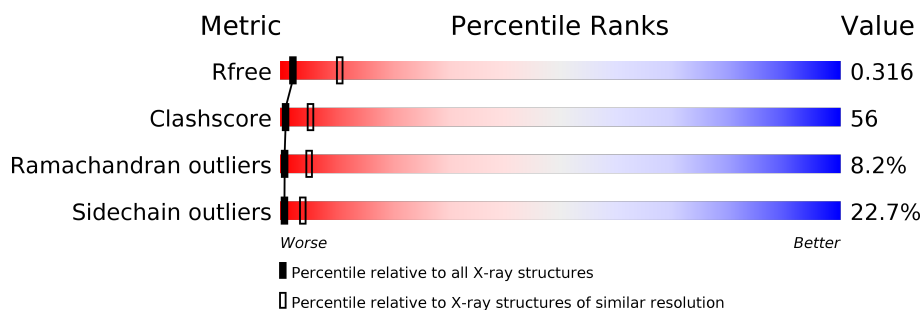
1 Overall quality at a glance

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 on 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 $\leq 5\%$.

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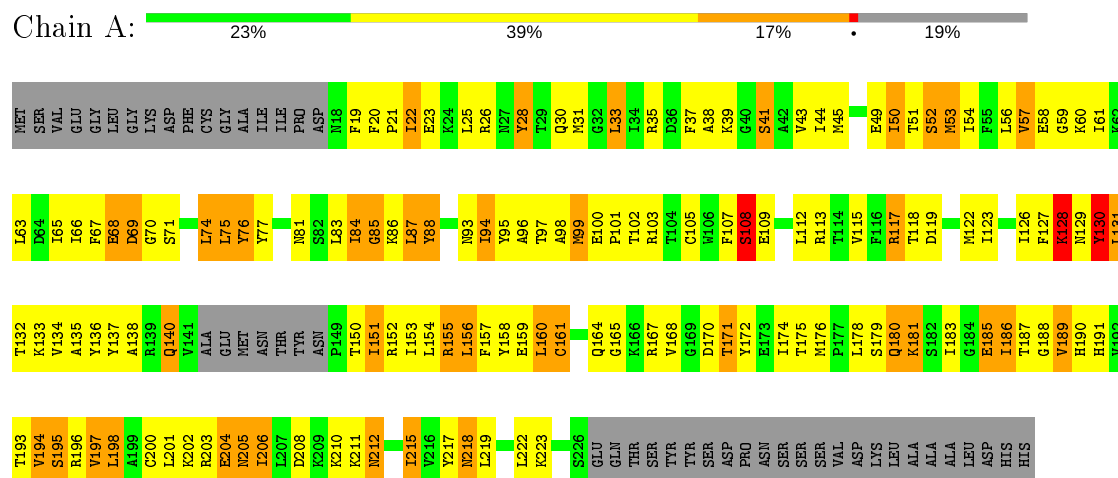
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Chain	Residue	Modelled	Actual	Comment	Reference
F	244	ALA	-	EXPRESSION TAG	UNP Q18R04
F	245	ALA	-	EXPRESSION TAG	UNP Q18R04
F	246	ALA	-	EXPRESSION TAG	UNP Q18R04
F	247	LEU	-	EXPRESSION TAG	UNP Q18R04
F	248	ASP	-	EXPRESSION TAG	UNP Q18R04
F	249	HIS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

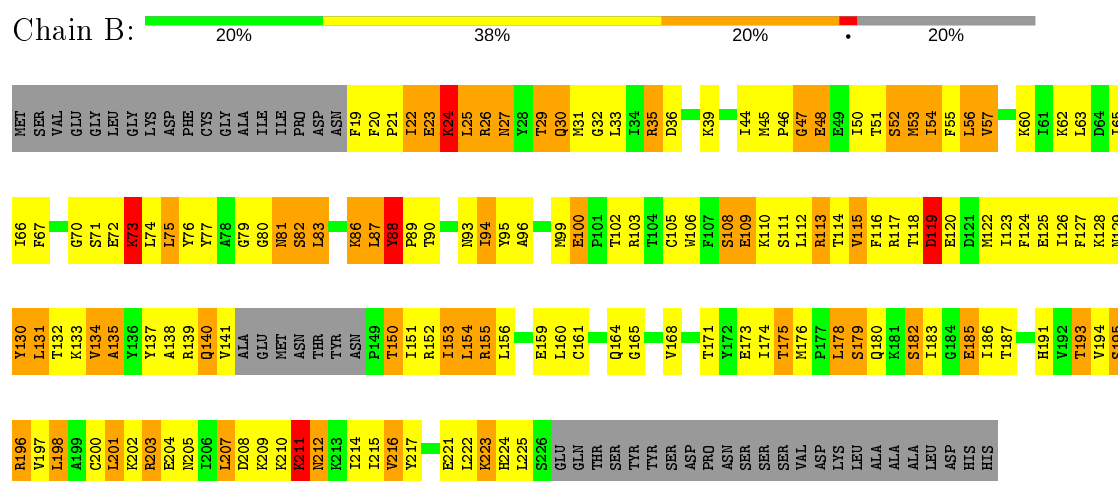
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

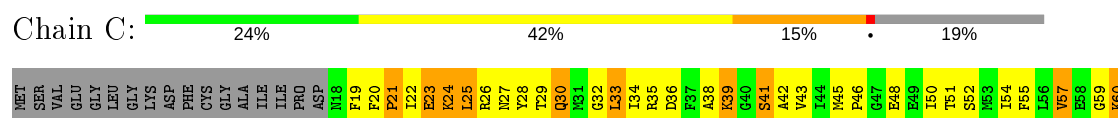
• Molecule 1: Cyclic nucleotide-binding protein

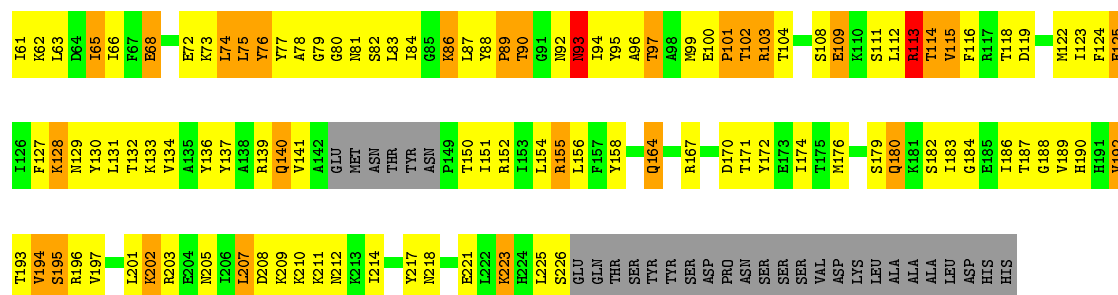


• Molecule 1: Cyclic nucleotide-binding protein

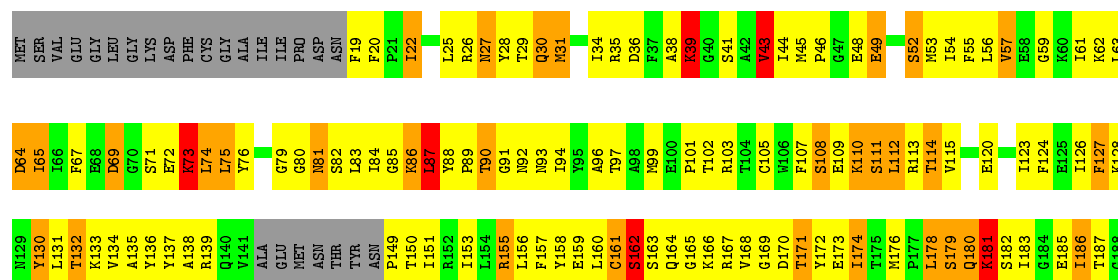
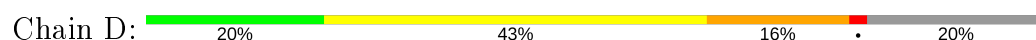


• Molecule 1: Cyclic nucleotide-binding protein

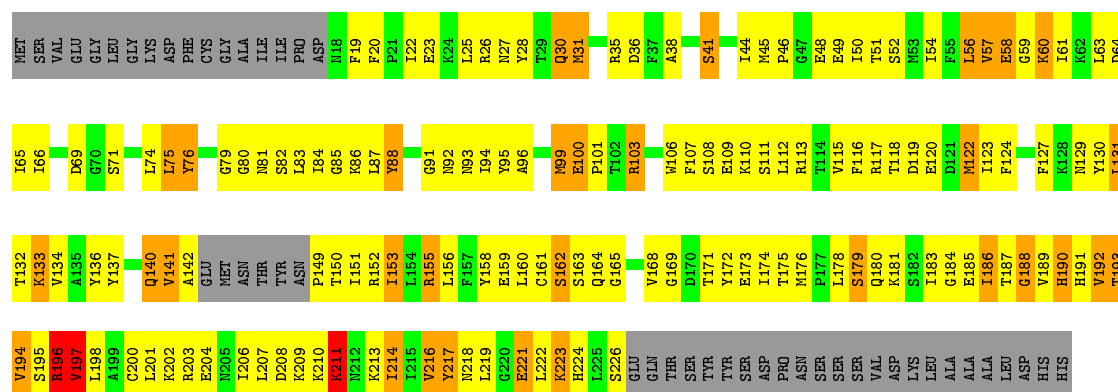
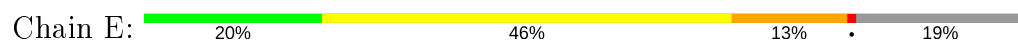




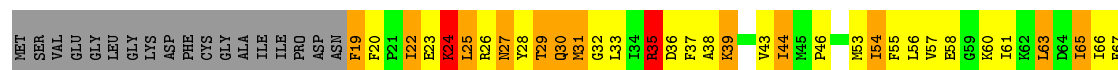
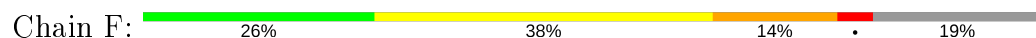
• Molecule 1: Cyclic nucleotide-binding protein



• Molecule 1: Cyclic nucleotide-binding protein



• Molecule 1: Cyclic nucleotide-binding protein



K208	K210	K211	K212	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	GLU	GLN	THR	SER	TYR	TYR	ASP	ASP	PRO	ASN	ASN	SER	SER	SER	SER	VAL	LYS	LEU	ALA	ALA	ALA	LEU	ASP	HIS	HIS												
R139	Q140	V141	E142	E143	MEP	ASN	THR	ASN	P149	R152	I153	I154	R155	L156	F157	I160	C161	S162	S163	R167	Y172	E173	I174	L178	S179	S182	I183	G184	E185	I186	T187	G188	H189	H190	H191	V192	T193	R196	V197	L198	A199	C200	L201	K202	R203	E204	N205	I206	L207	R208		
D58	D59	S71	E72	K73	L74	L75	Y76	Y77	A78	G79	S82	L83	I84	G85	R86	L87	Y88	N93	I94	Y95	A96	N99	E100	P101	T102	R103	T104	F107	S108	E109	K110	S111	L112	R113	T114	V115	E120	D121	M122	I123	F124	I125	L126	F127	K128	N129	Y130	V134	A135	Y136	L137	R138

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) 70.4 (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 0.321 , 0.316	Depositor DCC
R_{free} test set	1715 reflections (10.00%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	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 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	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	4
1	B	197/250 (79%)	146 (74%)	31 (16%)	20 (10%)	0	3
1	C	199/250 (80%)	151 (76%)	36 (18%)	12 (6%)	1	12
1	D	197/250 (79%)	144 (73%)	31 (16%)	22 (11%)	0	2
1	E	199/250 (80%)	152 (76%)	34 (17%)	13 (6%)	1	10
1	F	199/250 (80%)	156 (78%)	29 (15%)	14 (7%)	1	8
All	All	1189/1500 (79%)	889 (75%)	202 (17%)	98 (8%)	1	5

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	4
1	B	174/220 (79%)	133 (76%)	41 (24%)	1	3
1	C	170/220 (77%)	130 (76%)	40 (24%)	1	3
1	D	173/220 (79%)	134 (78%)	39 (22%)	1	4
1	E	170/220 (77%)	137 (81%)	33 (19%)	1	7
1	F	172/220 (78%)	130 (76%)	42 (24%)	0	2
All	All	1029/1320 (78%)	795 (77%)	234 (23%)	1	4

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 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 carbohydrates 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.