



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:41 PM UTC

PDB ID : 3E5Q / pdb_00003e5q
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

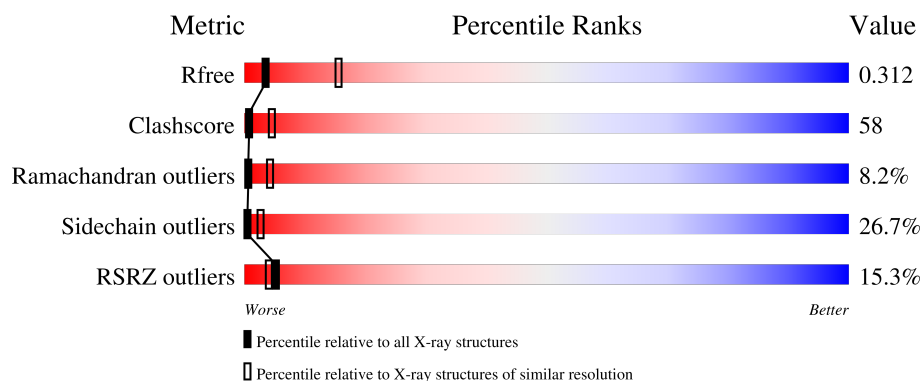
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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 $\leq 5\%$. 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	15% 19% 34% 22% 5% 19%
1	B	250	11% 17% 36% 22% 5% 20%
1	C	250	17% 22% 37% 19% • 19%
1	D	250	13% 18% 40% 20% • 20%
1	E	250	10% 18% 42% 19% • 19%

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Mol	Chain	Length	Quality of chain
1	F	250	8% 23% 37% 17% • 19%

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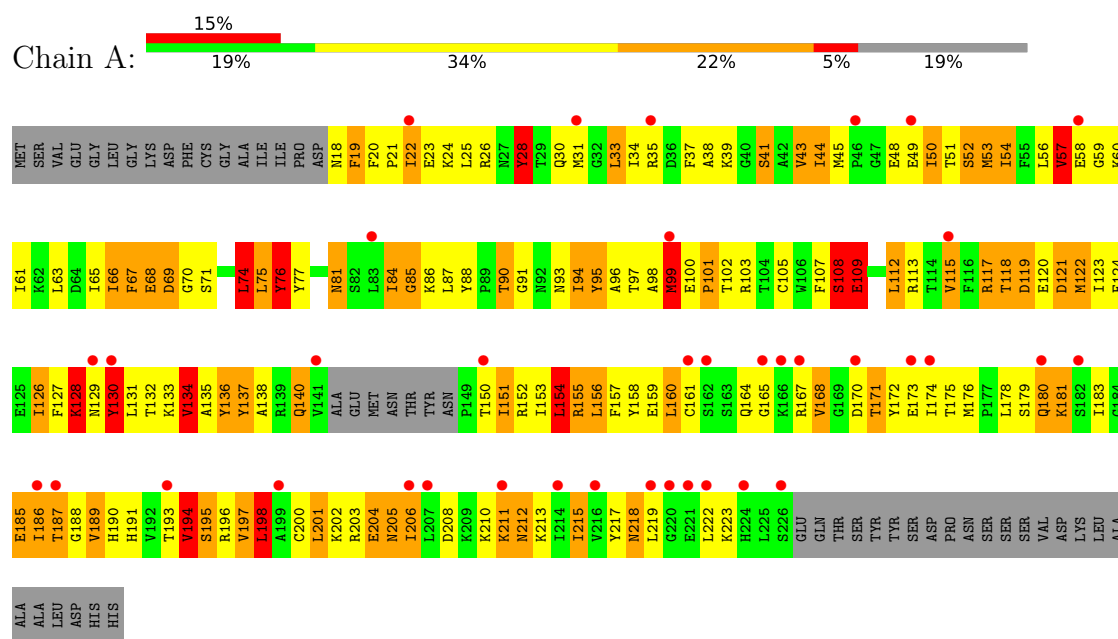
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Chain	Residue	Modelled	Actual	Comment	Reference
F	244	ALA	-	expression tag	UNP Q18R04
F	245	ALA	-	expression tag	UNP Q18R04
F	246	ALA	-	expression tag	UNP Q18R04
F	247	LEU	-	expression tag	UNP Q18R04
F	248	ASP	-	expression tag	UNP Q18R04
F	249	HIS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

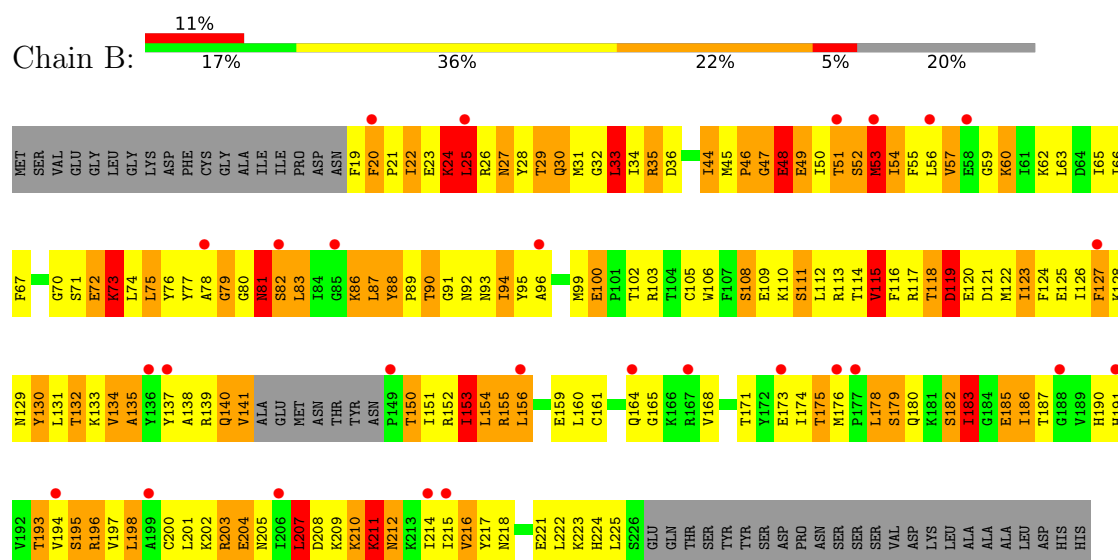
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: Cyclic nucleotide-binding protein



• Molecule 1: Cyclic nucleotide-binding protein



Chain C:

Amino Acid	Percentage
Met	17%
Val	22%
Leu	37%
Pro	19%
Asp	1%
Gly	19%

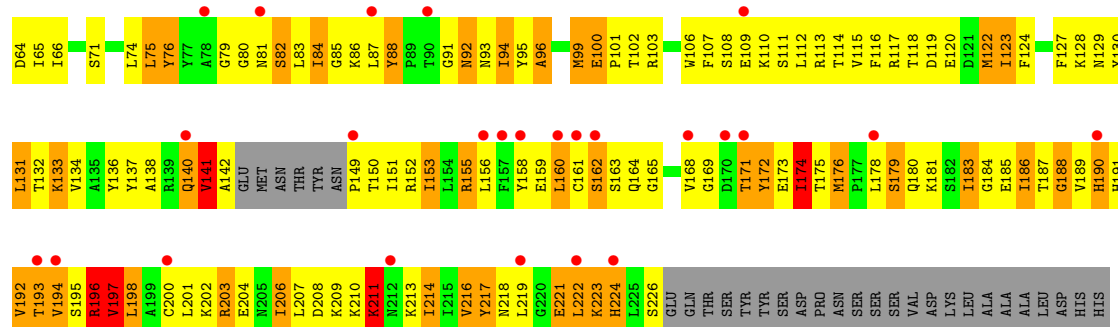
Chain D:

13% 18% 40% 20% 20%

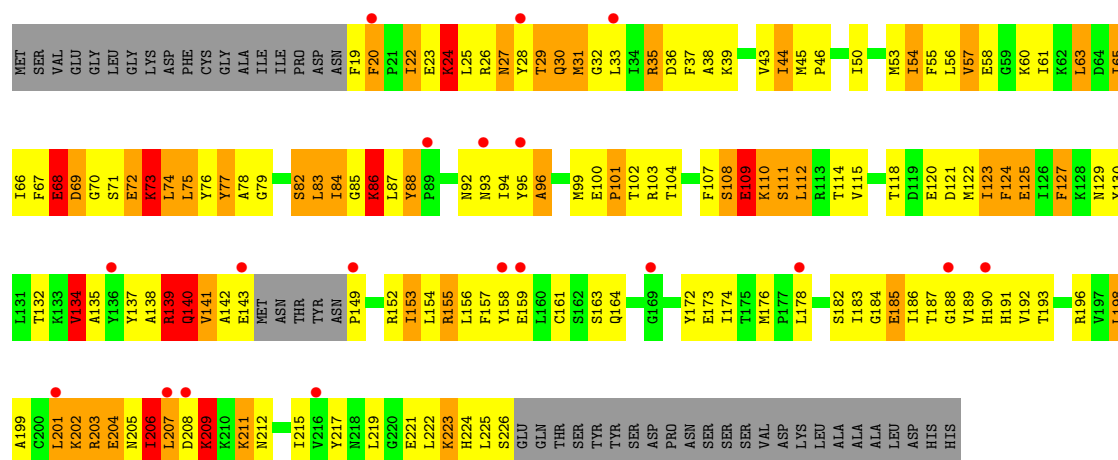
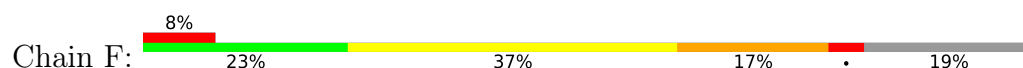
Amino Acid	Frequency
Met	1
Ser	1
Val	1
Glu	1
Gly	1
Leu	1
Gly	1
Lys	1
Asp	1
Phe	1
Cys	1
Gly	1
Ala	1
Ile	1
Pro	1
Asp	1
Asn	1
F19	1
F20	1
P21	1
I22	1
L25	1
R26	1
N27	1
Y28	1
T29	1
G30	1
N31	1
I34	1
R35	1
D36	1
F37	1
A38	1
R39	1
G40	1
S41	1
R103	1
A42	1
V43	1
I44	1
R45	1
P46	1
G47	1
E48	1
E49	1
S52	1
M53	1
I54	1
F55	1
L56	1
V57	1
E58	1
G59	1
R60	1
I61	1
E125	1
I126	1
K127	1
D64	1
I65	1
I66	1
VAL	1
F67	1
E68	1
D69	1
G70	1
S71	1
E72	1
K73	1
L74	1
L75	1
Y76	1
G79	1
G80	1
N81	1
S82	1
L83	1
I84	1
G85	1
K86	1
L87	1
Y88	1
P89	1
T90	1
G91	1
N92	1
N93	1
I94	1
Y95	1
A96	1
T97	1
A98	1
M99	1
E100	1
P101	1
T102	1
R103	1
T104	1
C105	1
I106	1
F107	1
S108	1
E109	1
K110	1
S111	1
L112	1
R113	1
T114	1
V115	1
E120	1
D121	1
M122	1
G123	1
F124	1
E125	1
I126	1
K127	1
K128	1
M129	1
Y130	1
L131	1
T132	1
K133	1
V134	1
A135	1
Y136	1
A137	1
A138	1
R139	1
Q140	1
V141	1
ALA	1
GLU	1
MET	1
ASN	1
THR	1
TYR	1
ASN	1
P149	1
T150	1
I151	1
R152	1
I153	1
L154	1
R155	1
L156	1
F157	1
Y158	1
E159	1
L160	1
C161	1
S162	1
S163	1
K164	1
G165	1
K166	1
R167	1
V168	1
G169	1
D170	1
T171	1
Y172	1
E173	1
I174	1
T175	1
M176	1
F177	1
L178	1
S179	1
Q180	1
K181	1
S182	1
I183	1
G184	1
E185	1
I186	1
T187	1
G188	1
V189	1
H190	1
H191	1
H192	1
T193	1
V194	1
L197	1
L198	1
A199	1
E200	1
K202	1
R203	1
E204	1
N205	1
L206	1
D207	1
D208	1
K209	1
K210	1
K211	1
N212	1
K213	1
I214	1
I215	1
V216	1
N218	1
L219	1
G220	1
E221	1
L222	1
K223	1
H224	1
L225	1
S226	1
GLU	1
GLN	1
THR	1
SER	1
TYR	1
TYR	1
SER	1
ASP	1
ASP	1
PRO	1
ASN	1
SER	1
SER	1
SER	1
VAL	1
ASP	1
LYS	

Chain E:

Amino Acid	Percentage
MET	10%
SER	18%
VAL	42%
GLU	19%
GLY	19%
LEU	
GLY	
LYS	
ASP	
PHE	
CYS	
GLY	
ALA	
ILE	
ILE	
PRO	
ASP	
R18	
F19	
F20	
P21	
I22	
E23	
K24	
L25	
R26	
N27	
Y28	
T29	
Q30	
R31	
G32	
R35	
D36	
F37	
A38	
S41	
I44	
M45	
P46	
G47	
E48	
E49	
I50	
T51	
S52	
M53	
I54	
F55	
L56	
V57	
E58	
G59	
K60	
I61	
K62	
K63	



● Molecule 1: Cyclic nucleotide-binding protein



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 – 3.20 142.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	79.8 (142.86-3.20) 70.4 (142.86-3.20)	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 0.319 , 0.312	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 , 58.8	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	1.39	7/1630 (0.4%)	1.60	26/2200 (1.2%)
1	B	1.47	12/1641 (0.7%)	1.61	24/2209 (1.1%)
1	C	1.22	4/1635 (0.2%)	1.52	29/2207 (1.3%)
1	D	1.14	2/1635 (0.1%)	1.35	14/2202 (0.6%)
1	E	1.19	5/1635 (0.3%)	1.50	23/2207 (1.0%)
1	F	1.15	4/1645 (0.2%)	1.42	19/2215 (0.9%)
All	All	1.27	34/9821 (0.3%)	1.50	135/13240 (1.0%)

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 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	TYR	CA-C	-8.73	1.42	1.52
1	B	90	THR	N-CA	6.88	1.54	1.46
1	F	134	VAL	CA-CB	-6.83	1.47	1.54
1	B	90	THR	CA-CB	6.63	1.62	1.53
1	B	33	LEU	CA-C	-6.34	1.44	1.52

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	TYR	N-CA-C	-10.52	96.04	108.14
1	B	118	THR	N-CA-C	-9.89	100.05	113.30
1	B	20	PHE	CA-C-N	9.41	131.60	119.84
1	B	20	PHE	C-N-CA	9.41	131.60	119.84
1	F	88	TYR	CA-C-N	9.24	129.28	119.76

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	218	0
1	B	1611	0	1643	239	0
1	C	1605	0	1606	200	0
1	D	1605	0	1632	214	1
1	E	1605	0	1606	208	0
1	F	1615	0	1637	196	1
All	All	9641	0	9725	1133	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 58.

The worst 5 of 1133 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	1.13	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%)	0	3
1	B	197/250 (79%)	146 (74%)	31 (16%)	20 (10%)	0	2
1	C	199/250 (80%)	151 (76%)	36 (18%)	12 (6%)	1	10
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	8
1	F	199/250 (80%)	156 (78%)	29 (15%)	14 (7%)	1	6
All	All	1189/1500 (79%)	889 (75%)	202 (17%)	98 (8%)	0	4

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%)	118 (69%)	52 (31%)	0	1
1	B	174/220 (79%)	126 (72%)	48 (28%)	0	2
1	C	170/220 (77%)	130 (76%)	40 (24%)	1	4
1	D	173/220 (79%)	132 (76%)	41 (24%)	1	4
1	E	170/220 (77%)	124 (73%)	46 (27%)	0	2
1	F	172/220 (78%)	124 (72%)	48 (28%)	0	2
All	All	1029/1320 (78%)	754 (73%)	275 (27%)	0	3

5 of 275 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	30	GLN
1	F	57	VAL
1	F	163	SER
1	B	211	LYS
1	B	198	LEU

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

Mol	Chain	Res	Type
1	D	27	ASN
1	E	30	GLN
1	F	191	HIS
1	D	205	ASN
1	E	81	ASN

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	1.17	38 (18%) 3 2	74, 81, 85, 90	0
1	B	201/250 (80%)	1.06	27 (13%) 7 6	74, 79, 84, 87	0
1	C	203/250 (81%)	1.23	42 (20%) 2 2	73, 80, 85, 91	0
1	D	201/250 (80%)	1.13	33 (16%) 4 3	73, 80, 85, 89	0
1	E	203/250 (81%)	1.03	26 (12%) 7 6	75, 80, 84, 90	0
1	F	203/250 (81%)	0.82	19 (9%) 14 9	75, 80, 84, 87	0
All	All	1213/1500 (80%)	1.07	185 (15%) 5 4	73, 80, 85, 91	0

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	161	CYS	8.1
1	C	156	LEU	7.1
1	C	201	LEU	6.5
1	A	161	CYS	6.4
1	D	206	ILE	5.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.