



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:34 AM GMT

PDB ID : 3P5T  
Title : CFIm25-CFIm68 complex  
Authors : Li, H.; Tong, S.; Li, X.; Shi, H.; Gao, Y.; Ge, H.; Niu, L.; Teng, M.  
Deposited on : 2010-10-11  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

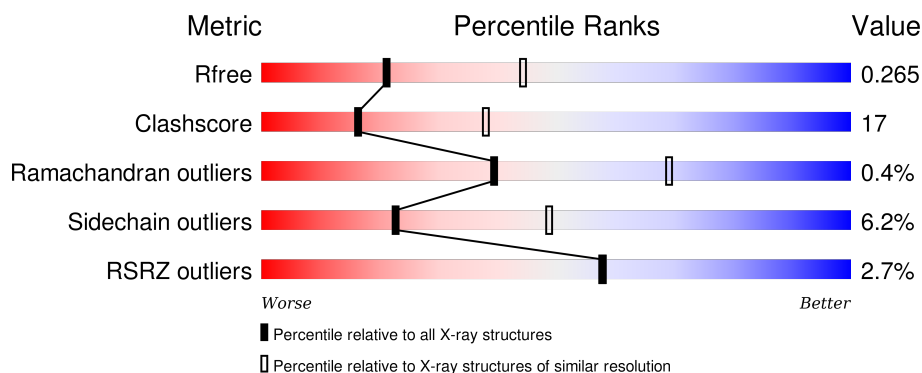
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	202	<div> <div>2%</div> <div>76% 18% . .</div> </div>
1	B	202	<div> <div>72% 24% . .</div> </div>
1	C	202	<div> <div>5%</div> <div>68% 26% . .</div> </div>
1	D	202	<div> <div>3%</div> <div>70% 24% . .</div> </div>
1	E	202	<div> <div>2%</div> <div>69% 21% . 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	202	<div><div></div><div>3%63%31%. .</div></div>
2	L	90	<div><div></div><div>7%50%29%. .16%</div></div>
2	M	90	<div><div></div><div>%69%20%.10%</div></div>
2	N	90	<div><div></div><div>68%20%.11%</div></div>
2	O	90	<div><div></div><div>67%20%.10%</div></div>
2	P	90	<div><div></div><div>57%26%6%12%</div></div>
2	Q	90	<div><div></div><div>6%61%24%.11%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13253 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 Cleavage and polyadenylation specificity factor subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1589	1037	270	278	4			
1	B	198	Total	C	N	O	S	0	0	0
			1611	1048	273	286	4			
1	C	196	Total	C	N	O	S	0	0	0
			1574	1028	264	278	4			
1	D	198	Total	C	N	O	S	0	0	0
			1613	1052	272	285	4			
1	E	191	Total	C	N	O	S	0	0	0
			1519	994	253	268	4			
1	F	197	Total	C	N	O	S	0	0	0
			1597	1041	270	282	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	LEU	-	EXPRESSION TAG	UNP O43809
A	229	GLU	-	EXPRESSION TAG	UNP O43809
A	230	HIS	-	EXPRESSION TAG	UNP O43809
A	231	HIS	-	EXPRESSION TAG	UNP O43809
A	232	HIS	-	EXPRESSION TAG	UNP O43809
A	233	HIS	-	EXPRESSION TAG	UNP O43809
A	234	HIS	-	EXPRESSION TAG	UNP O43809
A	235	HIS	-	EXPRESSION TAG	UNP O43809
B	228	LEU	-	EXPRESSION TAG	UNP O43809
B	229	GLU	-	EXPRESSION TAG	UNP O43809
B	230	HIS	-	EXPRESSION TAG	UNP O43809
B	231	HIS	-	EXPRESSION TAG	UNP O43809
B	232	HIS	-	EXPRESSION TAG	UNP O43809
B	233	HIS	-	EXPRESSION TAG	UNP O43809
B	234	HIS	-	EXPRESSION TAG	UNP O43809
B	235	HIS	-	EXPRESSION TAG	UNP O43809
C	228	LEU	-	EXPRESSION TAG	UNP O43809

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Chain	Residue	Modelled	Actual	Comment	Reference
C	229	GLU	-	EXPRESSION TAG	UNP O43809
C	230	HIS	-	EXPRESSION TAG	UNP O43809
C	231	HIS	-	EXPRESSION TAG	UNP O43809
C	232	HIS	-	EXPRESSION TAG	UNP O43809
C	233	HIS	-	EXPRESSION TAG	UNP O43809
C	234	HIS	-	EXPRESSION TAG	UNP O43809
C	235	HIS	-	EXPRESSION TAG	UNP O43809
D	228	LEU	-	EXPRESSION TAG	UNP O43809
D	229	GLU	-	EXPRESSION TAG	UNP O43809
D	230	HIS	-	EXPRESSION TAG	UNP O43809
D	231	HIS	-	EXPRESSION TAG	UNP O43809
D	232	HIS	-	EXPRESSION TAG	UNP O43809
D	233	HIS	-	EXPRESSION TAG	UNP O43809
D	234	HIS	-	EXPRESSION TAG	UNP O43809
D	235	HIS	-	EXPRESSION TAG	UNP O43809
E	228	LEU	-	EXPRESSION TAG	UNP O43809
E	229	GLU	-	EXPRESSION TAG	UNP O43809
E	230	HIS	-	EXPRESSION TAG	UNP O43809
E	231	HIS	-	EXPRESSION TAG	UNP O43809
E	232	HIS	-	EXPRESSION TAG	UNP O43809
E	233	HIS	-	EXPRESSION TAG	UNP O43809
E	234	HIS	-	EXPRESSION TAG	UNP O43809
E	235	HIS	-	EXPRESSION TAG	UNP O43809
F	228	LEU	-	EXPRESSION TAG	UNP O43809
F	229	GLU	-	EXPRESSION TAG	UNP O43809
F	230	HIS	-	EXPRESSION TAG	UNP O43809
F	231	HIS	-	EXPRESSION TAG	UNP O43809
F	232	HIS	-	EXPRESSION TAG	UNP O43809
F	233	HIS	-	EXPRESSION TAG	UNP O43809
F	234	HIS	-	EXPRESSION TAG	UNP O43809
F	235	HIS	-	EXPRESSION TAG	UNP O43809

- Molecule 2 is a protein called Cleavage and polyadenylation specificity factor subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	76	Total	C	N	O	S	0	0	0
			527	337	92	97	1			
2	M	81	Total	C	N	O	S	0	0	0
			603	385	100	117	1			
2	N	80	Total	C	N	O	S	0	0	0
			604	386	103	114	1			
2	O	81	Total	C	N	O	S	0	0	0
			599	382	98	118	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	79	Total	C	N	O	S	0	0	0
			586	375	97	113	1			
2	Q	80	Total	C	N	O	S	0	0	0
			583	372	97	113	1			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
L	162	LEU	-	EXPRESSION TAG	UNP Q16630
L	163	GLU	-	EXPRESSION TAG	UNP Q16630
L	164	HIS	-	EXPRESSION TAG	UNP Q16630
L	165	HIS	-	EXPRESSION TAG	UNP Q16630
L	166	HIS	-	EXPRESSION TAG	UNP Q16630
L	167	HIS	-	EXPRESSION TAG	UNP Q16630
L	168	HIS	-	EXPRESSION TAG	UNP Q16630
L	169	HIS	-	EXPRESSION TAG	UNP Q16630
M	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
M	162	LEU	-	EXPRESSION TAG	UNP Q16630
M	163	GLU	-	EXPRESSION TAG	UNP Q16630
M	164	HIS	-	EXPRESSION TAG	UNP Q16630
M	165	HIS	-	EXPRESSION TAG	UNP Q16630
M	166	HIS	-	EXPRESSION TAG	UNP Q16630
M	167	HIS	-	EXPRESSION TAG	UNP Q16630
M	168	HIS	-	EXPRESSION TAG	UNP Q16630
M	169	HIS	-	EXPRESSION TAG	UNP Q16630
N	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
N	162	LEU	-	EXPRESSION TAG	UNP Q16630
N	163	GLU	-	EXPRESSION TAG	UNP Q16630
N	164	HIS	-	EXPRESSION TAG	UNP Q16630
N	165	HIS	-	EXPRESSION TAG	UNP Q16630
N	166	HIS	-	EXPRESSION TAG	UNP Q16630
N	167	HIS	-	EXPRESSION TAG	UNP Q16630
N	168	HIS	-	EXPRESSION TAG	UNP Q16630
N	169	HIS	-	EXPRESSION TAG	UNP Q16630
O	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
O	162	LEU	-	EXPRESSION TAG	UNP Q16630
O	163	GLU	-	EXPRESSION TAG	UNP Q16630
O	164	HIS	-	EXPRESSION TAG	UNP Q16630
O	165	HIS	-	EXPRESSION TAG	UNP Q16630
O	166	HIS	-	EXPRESSION TAG	UNP Q16630
O	167	HIS	-	EXPRESSION TAG	UNP Q16630

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Chain	Residue	Modelled	Actual	Comment	Reference
O	168	HIS	-	EXPRESSION TAG	UNP Q16630
O	169	HIS	-	EXPRESSION TAG	UNP Q16630
P	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
P	162	LEU	-	EXPRESSION TAG	UNP Q16630
P	163	GLU	-	EXPRESSION TAG	UNP Q16630
P	164	HIS	-	EXPRESSION TAG	UNP Q16630
P	165	HIS	-	EXPRESSION TAG	UNP Q16630
P	166	HIS	-	EXPRESSION TAG	UNP Q16630
P	167	HIS	-	EXPRESSION TAG	UNP Q16630
P	168	HIS	-	EXPRESSION TAG	UNP Q16630
P	169	HIS	-	EXPRESSION TAG	UNP Q16630
Q	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
Q	162	LEU	-	EXPRESSION TAG	UNP Q16630
Q	163	GLU	-	EXPRESSION TAG	UNP Q16630
Q	164	HIS	-	EXPRESSION TAG	UNP Q16630
Q	165	HIS	-	EXPRESSION TAG	UNP Q16630
Q	166	HIS	-	EXPRESSION TAG	UNP Q16630
Q	167	HIS	-	EXPRESSION TAG	UNP Q16630
Q	168	HIS	-	EXPRESSION TAG	UNP Q16630
Q	169	HIS	-	EXPRESSION TAG	UNP Q16630

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	40	Total O 40 40	0	0
3	C	23	Total O 23 23	0	0
3	D	49	Total O 49 49	0	0
3	E	13	Total O 13 13	0	0
3	F	27	Total O 27 27	0	0
3	L	3	Total O 3 3	0	0
3	M	16	Total O 16 16	0	0
3	N	21	Total O 21 21	0	0

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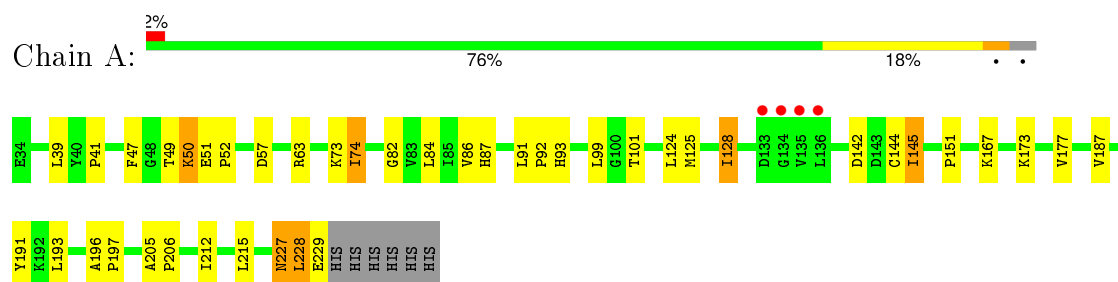
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	12	Total 12	O 12	0	0
3	P	6	Total 6	O 6	0	0
3	Q	8	Total 8	O 8	0	0



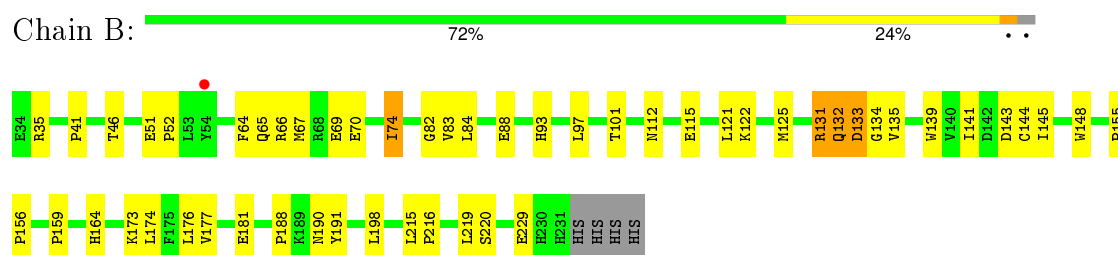
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

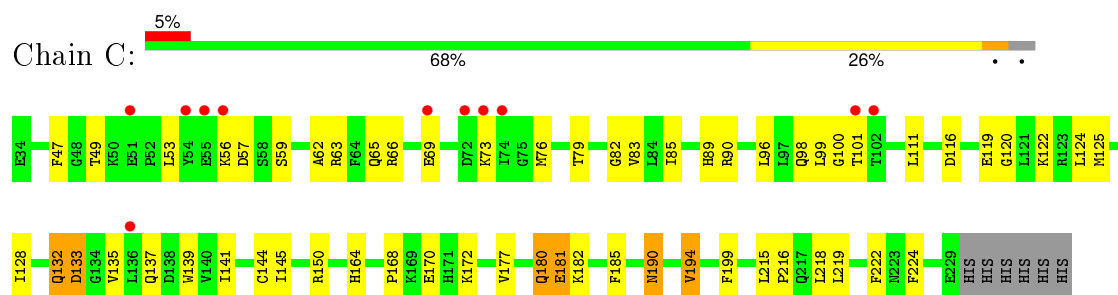
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5



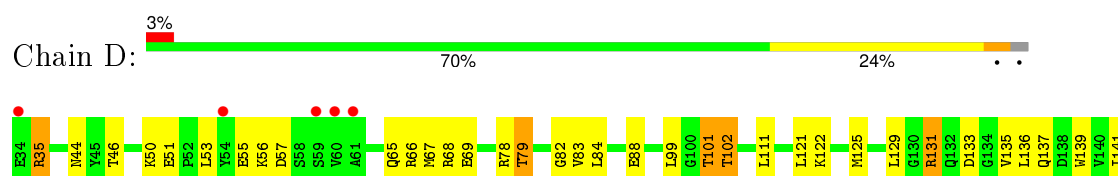
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

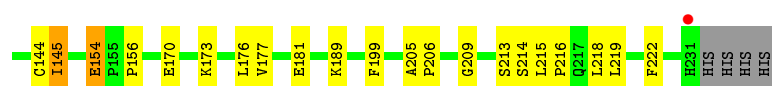


- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

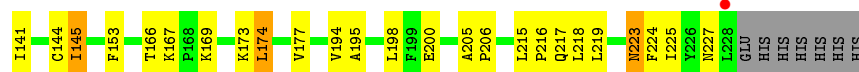


- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5





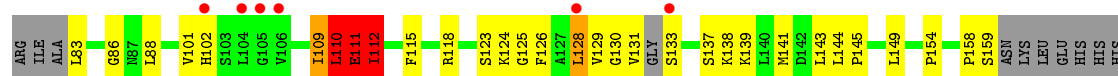
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5



- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



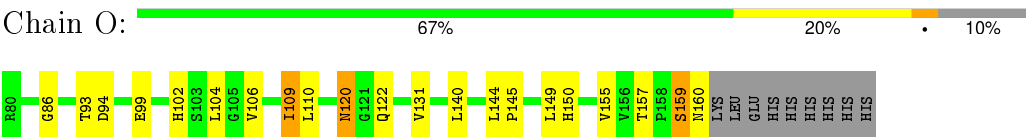
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



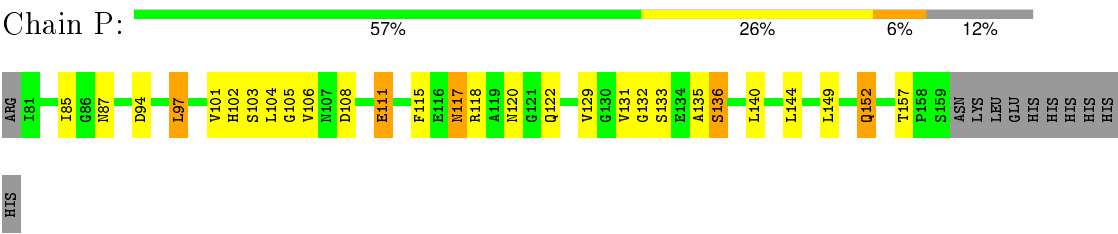
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



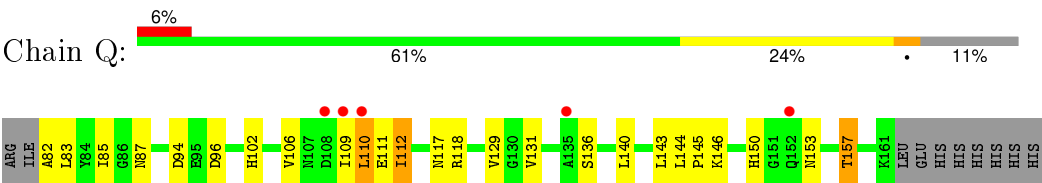
● Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



● Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



● Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.44Å 105.69Å 147.08Å 90.00° 112.72° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 29.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.70) 98.9 (29.94-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.29 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.214 , 0.265 0.213 , 0.265	Depositor DCC
$R_{free}$ test set	3101 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61654 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13253	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.49	0/1635	0.62	1/2223 (0.0%)
1	B	0.50	0/1658	0.63	0/2255
1	C	0.44	0/1620	0.62	0/2205
1	D	0.53	0/1661	0.67	1/2259 (0.0%)
1	E	0.43	0/1564	0.58	0/2133
1	F	0.45	0/1644	0.61	0/2238
2	L	0.57	0/537	0.97	4/735 (0.5%)
2	M	0.52	0/615	0.63	0/839
2	N	0.53	0/616	0.68	0/838
2	O	0.56	0/611	0.72	2/835 (0.2%)
2	P	0.51	0/598	0.65	0/816
2	Q	0.56	0/595	0.67	0/812
All	All	0.49	0/13354	0.65	8/18188 (0.0%)

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	F	0	1
2	L	1	2
All	All	1	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	112	ILE	CG1-CB-CG2	9.27	131.78	111.40
2	L	110	LEU	O-C-N	-9.20	107.98	122.70
2	L	112	ILE	CB-CA-C	-8.97	93.66	111.60
2	O	109	ILE	CB-CA-C	-7.03	97.55	111.60
1	D	219	LEU	CA-CB-CG	5.76	128.56	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	L	112	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	132	GLN	Peptide
2	L	110	LEU	Mainchain
2	L	111	GLU	Mainchain

## 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	1589	0	1578	33	0
1	B	1611	0	1586	56	0
1	C	1574	0	1547	54	0
1	D	1613	0	1594	50	0
1	E	1519	0	1471	47	0
1	F	1597	0	1563	69	0
2	L	527	0	446	32	0
2	M	603	0	573	11	0
2	N	604	0	589	14	0
2	O	599	0	564	13	0
2	P	586	0	553	33	0
2	Q	583	0	536	27	0
3	A	30	0	0	1	0
3	B	40	0	0	0	0
3	C	23	0	0	0	0
3	D	49	0	0	1	0
3	E	13	0	0	1	0
3	F	27	0	0	0	0
3	L	3	0	0	0	0
3	M	16	0	0	0	0
3	N	21	0	0	0	0
3	O	12	0	0	0	0
3	P	6	0	0	0	0
3	Q	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13253	0	12600	427	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 17.

The worst 5 of 427 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)
2:L:128:LEU:HD12	2:L:129:VAL:N	1.27	1.41
2:P:117:ASN:ND2	2:P:120:ASN:HB2	1.40	1.36
2:L:128:LEU:HD12	2:L:128:LEU:C	1.47	1.21
2:L:110:LEU:N	2:L:130:GLY:O	1.71	1.21
2:P:117:ASN:HD21	2:P:120:ASN:CB	1.55	1.17

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	194/202 (96%)	188 (97%)	6 (3%)	0	100	100
1	B	196/202 (97%)	187 (95%)	8 (4%)	1 (0%)	34	63
1	C	194/202 (96%)	186 (96%)	7 (4%)	1 (0%)	34	63
1	D	196/202 (97%)	184 (94%)	12 (6%)	0	100	100
1	E	187/202 (93%)	174 (93%)	12 (6%)	1 (0%)	34	63
1	F	195/202 (96%)	181 (93%)	13 (7%)	1 (0%)	34	63
2	L	72/90 (80%)	64 (89%)	7 (10%)	1 (1%)	14	35
2	M	79/90 (88%)	77 (98%)	1 (1%)	1 (1%)	15	37
2	N	78/90 (87%)	77 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	79/90 (88%)	75 (95%)	4 (5%)	0	100	100
2	P	77/90 (86%)	72 (94%)	4 (5%)	1 (1%)	15	37
2	Q	78/90 (87%)	70 (90%)	8 (10%)	0	100	100
All	All	1625/1752 (93%)	1535 (94%)	83 (5%)	7 (0%)	39	69

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	ASP
1	C	181	GLU
2	L	110	LEU
2	M	103	SER
2	P	103	SER

### 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	169/181 (93%)	159 (94%)	10 (6%)	24	51
1	B	172/181 (95%)	165 (96%)	7 (4%)	37	69
1	C	166/181 (92%)	159 (96%)	7 (4%)	36	68
1	D	173/181 (96%)	163 (94%)	10 (6%)	25	52
1	E	158/181 (87%)	147 (93%)	11 (7%)	19	42
1	F	168/181 (93%)	157 (94%)	11 (6%)	21	46
2	L	43/78 (55%)	37 (86%)	6 (14%)	4	10
2	M	62/78 (80%)	57 (92%)	5 (8%)	15	33
2	N	63/78 (81%)	62 (98%)	1 (2%)	70	91
2	O	62/78 (80%)	59 (95%)	3 (5%)	31	62
2	P	59/78 (76%)	52 (88%)	7 (12%)	6	15
2	Q	57/78 (73%)	51 (90%)	6 (10%)	8	19
All	All	1352/1554 (87%)	1268 (94%)	84 (6%)	23	49



5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	78	ARG
1	F	74	ILE
2	P	157	THR
1	E	99	LEU
1	E	174	LEU

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

Mol	Chain	Res	Type
2	L	153	ASN
2	M	122	GLN
2	Q	117	ASN
2	M	120	ASN
2	N	102	HIS

### 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 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	196/202 (97%)	-0.28	4 (2%) 68 69	14, 31, 48, 59	0
1	B	198/202 (98%)	-0.19	1 (0%) 91 93	16, 29, 54, 60	0
1	C	196/202 (97%)	0.15	11 (5%) 28 26	15, 42, 69, 77	0
1	D	198/202 (98%)	-0.21	6 (3%) 54 54	13, 24, 52, 61	0
1	E	191/202 (94%)	0.01	4 (2%) 67 68	24, 43, 76, 81	0
1	F	197/202 (97%)	-0.08	7 (3%) 46 46	23, 39, 70, 76	0
2	L	76/90 (84%)	0.63	6 (7%) 15 13	38, 63, 95, 98	0
2	M	81/90 (90%)	-0.15	1 (1%) 81 81	18, 33, 45, 47	0
2	N	80/90 (88%)	-0.32	0 100 100	18, 31, 37, 38	0
2	O	81/90 (90%)	-0.09	0 100 100	22, 36, 49, 51	0
2	P	79/90 (87%)	-0.03	0 100 100	26, 40, 56, 58	0
2	Q	80/90 (88%)	0.31	5 (6%) 23 22	36, 54, 66, 67	0
All	All	1653/1752 (94%)	-0.05	45 (2%) 58 58	13, 36, 67, 98	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	105	GLY	5.5
1	F	59	SER	5.1
1	C	54	TYR	4.7
1	D	60	VAL	4.4
1	D	54	TYR	4.1

### 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 carbohydrates 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.