



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 03:13 AM EDT

PDB ID : 3R84  
Title : Structure of the Mediator head subcomplex Med11/22  
Authors : Seizl, M.; Lariviere, L.; Pfaffenender, T.; Wenzek, L.; Cramer, P.  
Deposited on : 2011-03-23  
Resolution : 2.05 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

<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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

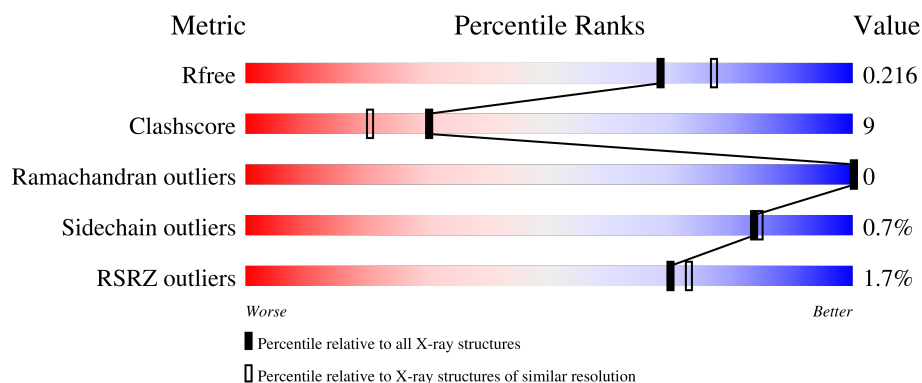
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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.















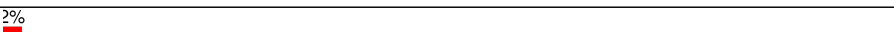

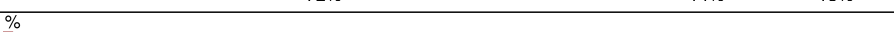




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	86	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 78%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>78%</span> <span>15%</span> <span>6%</span> </div> </div>
1	C	86	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 17%, green 74%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>74%</span> <span>17%</span> <span>7%</span> </div> </div>
1	E	86	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 10%, green 73%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>73%</span> <span>10%</span> <span>15%</span> </div> </div>
1	G	86	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 15%, green 77%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>77%</span> <span>15%</span> <span>8%</span> </div> </div>
1	I	86	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 1%, yellow 12%, green 81%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>81%</span> <span>12%</span> <span>7%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	86	
1	M	86	
1	O	86	
1	Q	86	
1	S	86	
1	U	86	
1	W	86	
2	B	92	
2	D	92	
2	F	92	
2	H	92	
2	J	92	
2	L	92	
2	N	92	
2	P	92	
2	R	92	
2	T	92	
2	V	92	
2	X	92	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16482 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 Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	Se	0	0	0
			666	419	116	129	1	1			
1	C	80	Total	C	N	O	S	Se	0	0	0
			658	413	115	128	1	1			
1	E	73	Total	C	N	O	S	Se	0	1	0
			617	388	106	121	1	1			
1	G	79	Total	C	N	O	S	Se	0	0	0
			651	408	114	127	1	1			
1	I	80	Total	C	N	O	S	Se	0	0	0
			658	413	115	128	1	1			
1	K	80	Total	C	N	O	S	Se	0	0	0
			658	413	115	128	1	1			
1	M	80	Total	C	N	O	S	Se	0	0	0
			658	413	115	128	1	1			
1	O	76	Total	C	N	O	S	Se	0	0	0
			624	390	108	124	1	1			
1	Q	80	Total	C	N	O	S	Se	0	0	0
			658	413	115	128	1	1			
1	S	81	Total	C	N	O	S	Se	0	0	0
			666	419	116	129	1	1			
1	U	81	Total	C	N	O	S	Se	0	0	0
			666	419	116	129	1	1			
1	W	73	Total	C	N	O	S	Se	0	0	0
			606	379	105	120	1	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	EXPRESSION TAG	UNP Q99278
C	4	GLY	-	EXPRESSION TAG	UNP Q99278
E	4	GLY	-	EXPRESSION TAG	UNP Q99278
G	4	GLY	-	EXPRESSION TAG	UNP Q99278
I	4	GLY	-	EXPRESSION TAG	UNP Q99278

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Chain	Residue	Modelled	Actual	Comment	Reference
K	4	GLY	-	EXPRESSION TAG	UNP Q99278
M	4	GLY	-	EXPRESSION TAG	UNP Q99278
O	4	GLY	-	EXPRESSION TAG	UNP Q99278
Q	4	GLY	-	EXPRESSION TAG	UNP Q99278
S	4	GLY	-	EXPRESSION TAG	UNP Q99278
U	4	GLY	-	EXPRESSION TAG	UNP Q99278
W	4	GLY	-	EXPRESSION TAG	UNP Q99278

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	80	Total	C	N	O	Se	0	3	0
			661	423	107	125	6			
2	D	79	Total	C	N	O	Se	0	3	0
			646	410	106	124	6			
2	F	77	Total	C	N	O	Se	0	3	0
			635	403	104	122	6			
2	H	79	Total	C	N	O	Se	0	2	0
			641	405	106	124	6			
2	J	79	Total	C	N	O	Se	0	2	0
			635	401	106	124	4			
2	L	79	Total	C	N	O	Se	0	3	0
			645	410	106	124	5			
2	N	80	Total	C	N	O	Se	0	3	0
			653	415	107	125	6			
2	P	77	Total	C	N	O	Se	0	2	0
			630	398	104	122	6			
2	R	79	Total	C	N	O	Se	0	4	0
			652	414	107	126	5			
2	T	79	Total	C	N	O	Se	0	3	0
			646	410	106	125	5			
2	V	81	Total	C	N	O	Se	0	2	0
			652	414	107	127	4			
2	X	78	Total	C	N	O	Se	0	3	0
			636	404	105	123	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP P32570
B	-1	SER	-	EXPRESSION TAG	UNP P32570
B	0	HIS	-	EXPRESSION TAG	UNP P32570

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	EXPRESSION TAG	UNP P32570
B	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
D	-2	GLY	-	EXPRESSION TAG	UNP P32570
D	-1	SER	-	EXPRESSION TAG	UNP P32570
D	0	HIS	-	EXPRESSION TAG	UNP P32570
D	1	MSE	-	EXPRESSION TAG	UNP P32570
D	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
F	-2	GLY	-	EXPRESSION TAG	UNP P32570
F	-1	SER	-	EXPRESSION TAG	UNP P32570
F	0	HIS	-	EXPRESSION TAG	UNP P32570
F	1	MSE	-	EXPRESSION TAG	UNP P32570
F	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
H	-2	GLY	-	EXPRESSION TAG	UNP P32570
H	-1	SER	-	EXPRESSION TAG	UNP P32570
H	0	HIS	-	EXPRESSION TAG	UNP P32570
H	1	MSE	-	EXPRESSION TAG	UNP P32570
H	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
J	-2	GLY	-	EXPRESSION TAG	UNP P32570
J	-1	SER	-	EXPRESSION TAG	UNP P32570
J	0	HIS	-	EXPRESSION TAG	UNP P32570
J	1	MSE	-	EXPRESSION TAG	UNP P32570
J	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
L	-2	GLY	-	EXPRESSION TAG	UNP P32570
L	-1	SER	-	EXPRESSION TAG	UNP P32570
L	0	HIS	-	EXPRESSION TAG	UNP P32570
L	1	MSE	-	EXPRESSION TAG	UNP P32570
L	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
N	-2	GLY	-	EXPRESSION TAG	UNP P32570
N	-1	SER	-	EXPRESSION TAG	UNP P32570
N	0	HIS	-	EXPRESSION TAG	UNP P32570
N	1	MSE	-	EXPRESSION TAG	UNP P32570
N	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
P	-2	GLY	-	EXPRESSION TAG	UNP P32570
P	-1	SER	-	EXPRESSION TAG	UNP P32570
P	0	HIS	-	EXPRESSION TAG	UNP P32570
P	1	MSE	-	EXPRESSION TAG	UNP P32570
P	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
R	-2	GLY	-	EXPRESSION TAG	UNP P32570
R	-1	SER	-	EXPRESSION TAG	UNP P32570
R	0	HIS	-	EXPRESSION TAG	UNP P32570
R	1	MSE	-	EXPRESSION TAG	UNP P32570
R	27	ILE	MET	ENGINEERED MUTATION	UNP P32570

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-2	GLY	-	EXPRESSION TAG	UNP P32570
T	-1	SER	-	EXPRESSION TAG	UNP P32570
T	0	HIS	-	EXPRESSION TAG	UNP P32570
T	1	MSE	-	EXPRESSION TAG	UNP P32570
T	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
V	-2	GLY	-	EXPRESSION TAG	UNP P32570
V	-1	SER	-	EXPRESSION TAG	UNP P32570
V	0	HIS	-	EXPRESSION TAG	UNP P32570
V	1	MSE	-	EXPRESSION TAG	UNP P32570
V	27	ILE	MET	ENGINEERED MUTATION	UNP P32570
X	-2	GLY	-	EXPRESSION TAG	UNP P32570
X	-1	SER	-	EXPRESSION TAG	UNP P32570
X	0	HIS	-	EXPRESSION TAG	UNP P32570
X	1	MSE	-	EXPRESSION TAG	UNP P32570
X	27	ILE	MET	ENGINEERED MUTATION	UNP P32570

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	35	Total O 35 35	0	0
3	B	47	Total O 47 47	0	0
3	C	29	Total O 29 29	0	0
3	D	43	Total O 43 43	0	0
3	E	46	Total O 46 46	0	0
3	F	39	Total O 39 39	0	0
3	G	41	Total O 41 41	0	0
3	H	40	Total O 40 40	0	0
3	I	38	Total O 38 38	0	0
3	J	42	Total O 42 42	0	0
3	K	44	Total O 44 44	0	0
3	L	38	Total O 38 38	0	0

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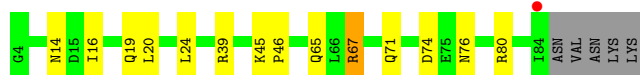
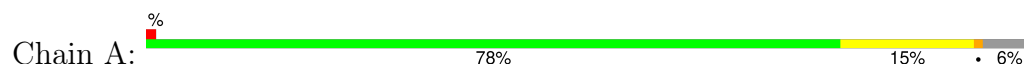
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	21	Total 21	O 21	0	0
3	N	43	Total 43	O 43	0	0
3	O	43	Total 43	O 43	0	0
3	P	42	Total 42	O 42	0	0
3	Q	27	Total 27	O 27	0	0
3	R	31	Total 31	O 31	0	0
3	S	29	Total 29	O 29	0	0
3	T	42	Total 42	O 42	0	0
3	U	50	Total 50	O 50	0	0
3	V	50	Total 50	O 50	0	0
3	W	65	Total 65	O 65	0	0
3	X	39	Total 39	O 39	0	0



### 3 Residue-property plots [i](#)

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: Mediator of RNA polymerase II transcription subunit 11



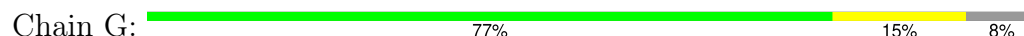
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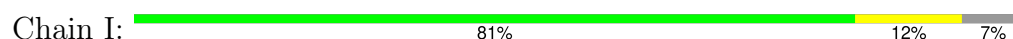
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11



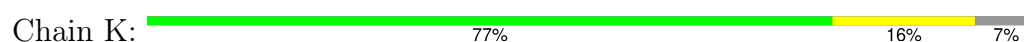
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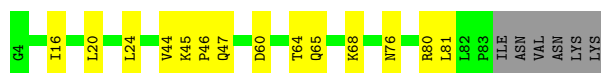


- Molecule 1: Mediator of RNA polymerase II transcription subunit 11

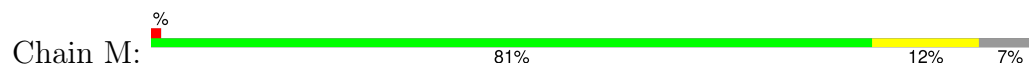


- Molecule 1: Mediator of RNA polymerase II transcription subunit 11





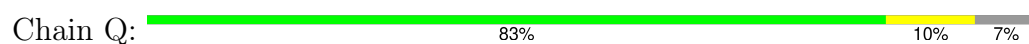
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11



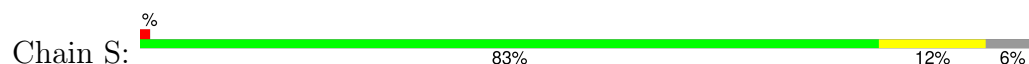
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11



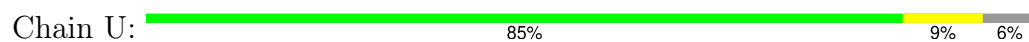
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11



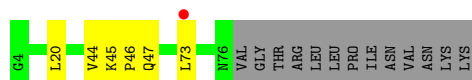
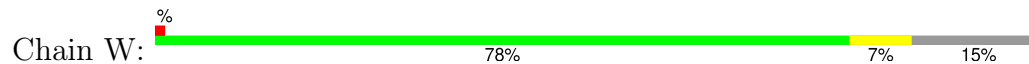
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11



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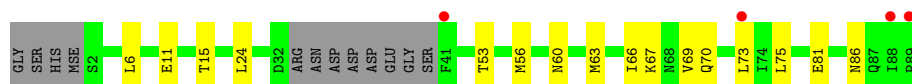


- Molecule 1: Mediator of RNA polymerase II transcription subunit 11

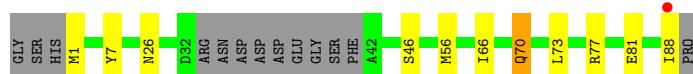
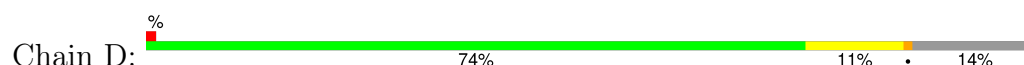


- Molecule 2: Mediator of RNA polymerase II transcription subunit 22

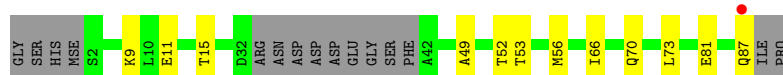




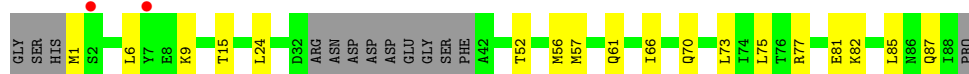
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



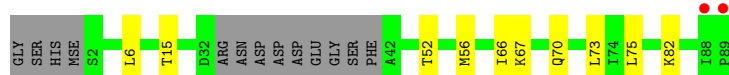
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



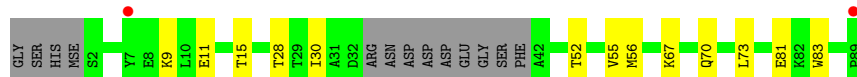
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



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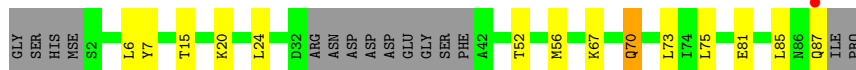
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



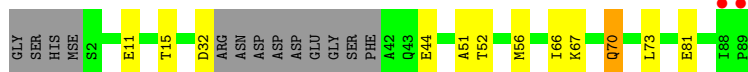
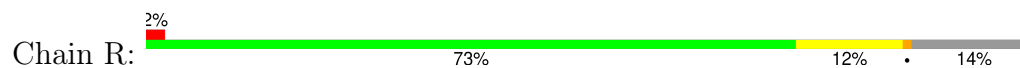
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



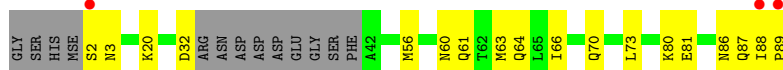
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



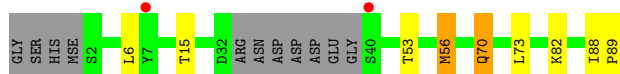
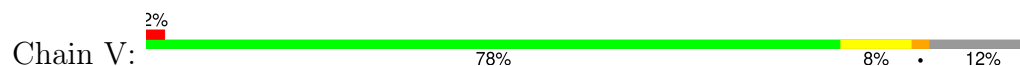
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



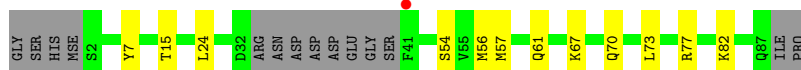
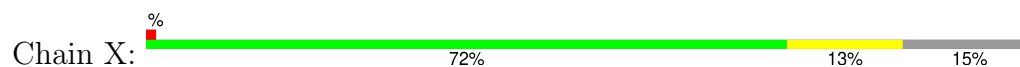
- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



- Molecule 2: Mediator of RNA polymerase II transcription subunit 22



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.49Å 173.79Å 101.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.04 – 2.05 83.86 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.9 (66.04-2.05) 99.7 (83.86-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.170 , 0.208 0.180 , 0.216	Depositor DCC
$R_{free}$ test set	8179 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16482	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.38	0/673	0.48	0/901
1	C	0.41	0/665	0.47	0/890
1	E	0.39	0/624	0.45	0/833
1	G	0.40	0/657	0.44	0/878
1	I	0.44	0/665	0.49	0/890
1	K	0.39	0/665	0.50	0/890
1	M	0.36	0/665	0.48	0/890
1	O	0.41	0/630	0.46	0/842
1	Q	0.37	0/665	0.46	0/890
1	S	0.40	0/673	0.45	0/901
1	U	0.45	0/673	0.52	0/901
1	W	0.44	0/612	0.48	0/817
2	B	0.41	0/673	0.53	0/898
2	D	0.38	0/654	0.53	0/873
2	F	0.38	0/645	0.51	0/859
2	H	0.41	0/646	0.53	0/862
2	J	0.41	0/639	0.53	0/857
2	L	0.39	0/654	0.51	0/875
2	N	0.39	0/662	0.52	0/885
2	P	0.39	0/637	0.51	0/848
2	R	0.38	0/664	0.51	0/887
2	T	0.40	0/655	0.50	0/875
2	V	0.46	0/657	0.53	0/880
2	X	0.44	0/643	0.56	0/861
All	All	0.40	0/15696	0.50	0/20983

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	666	0	674	16	0
1	C	658	0	663	14	0
1	E	617	0	610	12	0
1	G	651	0	656	12	0
1	I	658	0	663	8	0
1	K	658	0	663	13	0
1	M	658	0	663	10	0
1	O	624	0	621	15	0
1	Q	658	0	663	12	0
1	S	666	0	674	10	0
1	U	666	0	674	6	0
1	W	606	0	602	6	0
2	B	661	0	715	27	0
2	D	646	0	702	17	0
2	F	635	0	687	22	0
2	H	641	0	691	27	0
2	J	635	0	677	13	0
2	L	645	0	697	29	0
2	N	653	0	709	23	0
2	P	630	0	677	25	0
2	R	652	0	705	21	0
2	T	646	0	697	34	0
2	V	652	0	694	26	0
2	X	636	0	679	36	0
3	A	35	0	0	1	0
3	B	47	0	0	0	0
3	C	29	0	0	0	0
3	D	43	0	0	0	0
3	E	46	0	0	2	0
3	F	39	0	0	1	0
3	G	41	0	0	1	0
3	H	40	0	0	1	0
3	I	38	0	0	0	0
3	J	42	0	0	0	0
3	K	44	0	0	5	0
3	L	38	0	0	1	0
3	M	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	43	0	0	1	0
3	O	43	0	0	0	0
3	P	42	0	0	0	0
3	Q	27	0	0	1	0
3	R	31	0	0	0	0
3	S	29	0	0	1	0
3	T	42	0	0	3	0
3	U	50	0	0	1	0
3	V	50	0	0	0	0
3	W	65	0	0	1	0
3	X	39	0	0	0	0
All	All	16482	0	16156	294	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 9.

The worst 5 of 294 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:J:73:LEU:HD13	2:L:56[B]:MSE:SE	1.88	1.22
2:V:56[A]:MSE:SE	2:X:73[A]:LEU:HD22	1.89	1.22
2:T:2:SER:N	2:T:3:ASN:HA	1.71	1.05
2:B:70[B]:GLN:HE21	2:B:70[B]:GLN:HA	1.24	1.00
2:F:73[B]:LEU:HD22	2:H:56[B]:MSE:HE2	1.43	1.00

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	79/86 (92%)	78 (99%)	1 (1%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	78/86 (91%)	77 (99%)	1 (1%)	0	100	100
1	E	72/86 (84%)	72 (100%)	0	0	100	100
1	G	77/86 (90%)	76 (99%)	1 (1%)	0	100	100
1	I	78/86 (91%)	76 (97%)	2 (3%)	0	100	100
1	K	78/86 (91%)	77 (99%)	1 (1%)	0	100	100
1	M	78/86 (91%)	77 (99%)	1 (1%)	0	100	100
1	O	74/86 (86%)	74 (100%)	0	0	100	100
1	Q	78/86 (91%)	78 (100%)	0	0	100	100
1	S	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
1	U	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
1	W	71/86 (83%)	71 (100%)	0	0	100	100
2	B	81/92 (88%)	81 (100%)	0	0	100	100
2	D	79/92 (86%)	79 (100%)	0	0	100	100
2	F	78/92 (85%)	77 (99%)	1 (1%)	0	100	100
2	H	78/92 (85%)	77 (99%)	1 (1%)	0	100	100
2	J	77/92 (84%)	77 (100%)	0	0	100	100
2	L	79/92 (86%)	79 (100%)	0	0	100	100
2	N	80/92 (87%)	80 (100%)	0	0	100	100
2	P	77/92 (84%)	77 (100%)	0	0	100	100
2	R	80/92 (87%)	80 (100%)	0	0	100	100
2	T	79/92 (86%)	78 (99%)	1 (1%)	0	100	100
2	V	79/92 (86%)	79 (100%)	0	0	100	100
2	X	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
All	All	1865/2136 (87%)	1852 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	76/80 (95%)	74 (97%)	2 (3%)	46	39
1	C	75/80 (94%)	73 (97%)	2 (3%)	44	38
1	E	70/80 (88%)	69 (99%)	1 (1%)	67	65
1	G	74/80 (92%)	74 (100%)	0	100	100
1	I	75/80 (94%)	74 (99%)	1 (1%)	69	67
1	K	75/80 (94%)	75 (100%)	0	100	100
1	M	75/80 (94%)	75 (100%)	0	100	100
1	O	71/80 (89%)	70 (99%)	1 (1%)	67	65
1	Q	75/80 (94%)	75 (100%)	0	100	100
1	S	76/80 (95%)	76 (100%)	0	100	100
1	U	76/80 (95%)	76 (100%)	0	100	100
1	W	69/80 (86%)	69 (100%)	0	100	100
2	B	79/80 (99%)	79 (100%)	0	100	100
2	D	77/80 (96%)	75 (97%)	2 (3%)	46	39
2	F	76/80 (95%)	76 (100%)	0	100	100
2	H	76/80 (95%)	76 (100%)	0	100	100
2	J	75/80 (94%)	75 (100%)	0	100	100
2	L	77/80 (96%)	77 (100%)	0	100	100
2	N	78/80 (98%)	77 (99%)	1 (1%)	69	67
2	P	75/80 (94%)	73 (97%)	2 (3%)	44	38
2	R	78/80 (98%)	76 (97%)	2 (3%)	46	39
2	T	77/80 (96%)	77 (100%)	0	100	100
2	V	77/80 (96%)	74 (96%)	3 (4%)	32	25
2	X	75/80 (94%)	75 (100%)	0	100	100
All	All	1807/1920 (94%)	1790 (99%)	17 (1%)	84	79

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	V	56[A]	MSE
2	V	70	GLN
1	I	74	ASP
2	N	85	LEU
1	O	28	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	4	GLN
2	T	64	GLN
1	Q	76	ASN
2	T	4	GLN
1	U	47	GLN

### 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 monosaccharides 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 ⓘ

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	80/86 (93%)	-0.08	1 (1%) 77 79	21, 31, 60, 92	0
1	C	79/86 (91%)	-0.16	0 100 100	21, 35, 68, 92	0
1	E	72/86 (83%)	-0.20	0 100 100	20, 31, 48, 56	0
1	G	78/86 (90%)	-0.15	0 100 100	19, 32, 58, 94	0
1	I	79/86 (91%)	-0.24	0 100 100	18, 29, 50, 71	0
1	K	79/86 (91%)	-0.26	0 100 100	19, 29, 45, 76	0
1	M	79/86 (91%)	0.02	1 (1%) 77 79	22, 38, 73, 117	0
1	O	75/86 (87%)	-0.04	3 (4%) 38 41	20, 30, 49, 114	0
1	Q	79/86 (91%)	-0.09	0 100 100	20, 34, 61, 99	0
1	S	80/86 (93%)	-0.12	1 (1%) 77 79	17, 31, 58, 90	0
1	U	80/86 (93%)	-0.18	0 100 100	16, 27, 46, 67	0
1	W	72/86 (83%)	-0.22	1 (1%) 75 78	17, 25, 45, 63	0
2	B	77/92 (83%)	0.03	4 (5%) 27 29	19, 28, 58, 99	0
2	D	75/92 (81%)	-0.15	1 (1%) 77 79	17, 29, 56, 88	0
2	F	74/92 (80%)	-0.13	1 (1%) 75 78	20, 27, 54, 82	0
2	H	75/92 (81%)	-0.11	2 (2%) 54 59	17, 27, 65, 89	0
2	J	76/92 (82%)	-0.07	2 (2%) 56 60	18, 26, 55, 97	0
2	L	76/92 (82%)	-0.07	2 (2%) 56 60	19, 27, 56, 101	0
2	N	76/92 (82%)	-0.02	3 (3%) 39 42	20, 30, 63, 137	0
2	P	74/92 (80%)	-0.05	1 (1%) 75 78	19, 29, 53, 81	0
2	R	76/92 (82%)	-0.09	2 (2%) 56 60	20, 29, 58, 109	0
2	T	76/92 (82%)	-0.01	3 (3%) 39 42	16, 28, 61, 120	0
2	V	78/92 (84%)	-0.03	2 (2%) 56 60	16, 23, 56, 91	0
2	X	75/92 (81%)	-0.07	1 (1%) 77 79	18, 24, 55, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	1840/2136 (86%)	-0.10	31 (1%) 70 73	16, 29, 58, 137	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	89	PRO	5.2
1	O	79	THR	5.2
2	B	41	PHE	5.2
1	S	84	ILE	4.8
2	T	88	ILE	4.7

## 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 monosaccharides 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.