wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 01:11 pm BST

PDB ID	:	3RJ1
Title	:	Architecture of the Mediator Head module
Authors	:	Imasaki, T.; Calero, G.; Cai, G.; Tsai, K.L.; Yamada, K.; Cardelli, F.; Erdjument-Bromage, H.; Tempst, P.; Berger, I.; Kornberg, G.L.; Asturias, F.J.; Kornberg, R.D.; Takagi, Y.
Deposited on	:	2011-04-14
Resolution	:	4.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

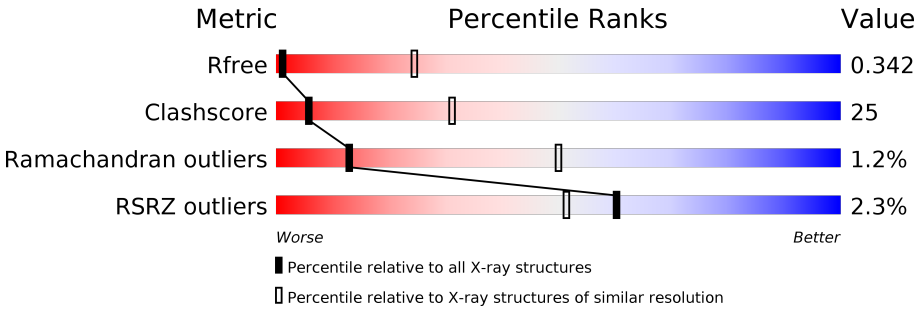
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 >=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 <=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	131	53% 18% 28%
1	H	131	55% 17% 28%
1	O	131	% 56% 15% 28%
2	B	583	% 45% 9% 45%
2	I	583	45% 9% • 45%
2	P	583	44% 10% 45%
3	C	223	48% 21% • 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	223	48% 22% 29%
3	Q	223	47% 22% 29%
4	D	121	46% 26% 27%
4	K	121	45% 28% 27%
4	R	121	47% 26% 27%
5	E	275	4% 63% 21% 16%
5	L	275	59% 25% 16%
5	S	275	4% 62% 22% 16%
6	F	210	14% 83% 15%
6	M	210	3% 81% 16%
6	T	210	4% 82% 16%
7	G	295	2% 25% 9% 65%
7	N	295	25% 9% 65%
7	U	295	25% 9% 65%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SE	B	1730	-	-	X	-
8	SE	B	904	-	-	-	X
8	SE	C	225	-	-	-	X
8	SE	D	1301	-	-	X	-
8	SE	D	222	-	-	X	-
8	SE	D	223	-	-	-	X
8	SE	E	409	-	-	X	-
8	SE	E	410	-	-	X	-
8	SE	G	1296	-	-	-	X
8	SE	H	313	-	-	-	X
8	SE	I	901	-	-	-	X
8	SE	I	904	-	-	-	X
8	SE	I	906	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SE	J	225	-	-	X	-
8	SE	K	174	-	-	X	-
8	SE	K	175	-	-	X	-
8	SE	K	177	-	-	X	-
8	SE	L	408	-	-	X	-
8	SE	L	412	-	-	-	X
8	SE	L	413	-	-	X	-
8	SE	L	414	-	-	-	X
8	SE	L	415	-	-	X	-
8	SE	N	397	-	-	-	X
8	SE	N	398	-	-	X	-
8	SE	O	132	-	-	X	-
8	SE	O	133	-	-	-	X
8	SE	P	1731	-	-	-	X
8	SE	P	1733	-	-	X	-
8	SE	Q	325	-	-	X	-
8	SE	S	309	-	-	-	X
8	SE	S	310	-	-	X	-
8	SE	S	311	-	-	-	X
8	SE	S	312	-	-	-	X
8	SE	U	499	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17945 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	94	Total	C	N	O	0	0	0
			468	280	94	94			
1	H	94	Total	C	N	O	0	0	0
			468	280	94	94			
1	O	94	Total	C	N	O	0	0	0
			468	280	94	94			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	THR	ENGINEERED MUTATION	UNP Q99278
A	17	SER	MET	ENGINEERED MUTATION	UNP Q99278
H	16	GLY	THR	ENGINEERED MUTATION	UNP Q99278
H	17	SER	MET	ENGINEERED MUTATION	UNP Q99278
O	16	GLY	THR	ENGINEERED MUTATION	UNP Q99278
O	17	SER	MET	ENGINEERED MUTATION	UNP Q99278

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	318	Total	C	N	O	0	0	0
			1583	947	318	318			
2	I	318	Total	C	N	O	0	0	0
			1583	947	318	318			
2	P	318	Total	C	N	O	0	0	0
			1583	947	318	318			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	MSE	-	EXPRESSION TAG	UNP P32569
B	99	HIS	-	EXPRESSION TAG	UNP P32569

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	HIS	-	EXPRESSION TAG	UNP P32569
B	101	HIS	-	EXPRESSION TAG	UNP P32569
B	102	HIS	-	EXPRESSION TAG	UNP P32569
B	103	HIS	-	EXPRESSION TAG	UNP P32569
B	104	HIS	-	EXPRESSION TAG	UNP P32569
B	105	HIS	-	EXPRESSION TAG	UNP P32569
B	106	HIS	-	EXPRESSION TAG	UNP P32569
B	107	HIS	-	EXPRESSION TAG	UNP P32569
B	108	HIS	-	EXPRESSION TAG	UNP P32569
I	98	MSE	-	EXPRESSION TAG	UNP P32569
I	99	HIS	-	EXPRESSION TAG	UNP P32569
I	100	HIS	-	EXPRESSION TAG	UNP P32569
I	101	HIS	-	EXPRESSION TAG	UNP P32569
I	102	HIS	-	EXPRESSION TAG	UNP P32569
I	103	HIS	-	EXPRESSION TAG	UNP P32569
I	104	HIS	-	EXPRESSION TAG	UNP P32569
I	105	HIS	-	EXPRESSION TAG	UNP P32569
I	106	HIS	-	EXPRESSION TAG	UNP P32569
I	107	HIS	-	EXPRESSION TAG	UNP P32569
I	108	HIS	-	EXPRESSION TAG	UNP P32569
P	98	MSE	-	EXPRESSION TAG	UNP P32569
P	99	HIS	-	EXPRESSION TAG	UNP P32569
P	100	HIS	-	EXPRESSION TAG	UNP P32569
P	101	HIS	-	EXPRESSION TAG	UNP P32569
P	102	HIS	-	EXPRESSION TAG	UNP P32569
P	103	HIS	-	EXPRESSION TAG	UNP P32569
P	104	HIS	-	EXPRESSION TAG	UNP P32569
P	105	HIS	-	EXPRESSION TAG	UNP P32569
P	106	HIS	-	EXPRESSION TAG	UNP P32569
P	107	HIS	-	EXPRESSION TAG	UNP P32569
P	108	HIS	-	EXPRESSION TAG	UNP P32569

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	159	Total	C	N	O	0	0	0
			791	473	159	159			
3	J	159	Total	C	N	O	0	0	0
			791	473	159	159			
3	Q	159	Total	C	N	O	0	0	0
			791	473	159	159			

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	88	Total	C	N	O	0	0	0
			440	264	88	88			
4	K	88	Total	C	N	O	0	0	0
			440	264	88	88			
4	R	88	Total	C	N	O	0	0	0
			440	264	88	88			

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	0	0	0
			1141	679	231	231			
5	L	231	Total	C	N	O	0	0	0
			1141	679	231	231			
5	S	231	Total	C	N	O	0	0	0
			1141	679	231	231			

- Molecule 6 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	205	Total	C	N	O	0	0	0
			1012	602	205	205			
6	M	205	Total	C	N	O	0	0	0
			1012	602	205	205			
6	T	205	Total	C	N	O	0	0	0
			1012	602	205	205			

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	103	Total	C	N	O	0	0	0
			514	308	103	103			
7	N	103	Total	C	N	O	0	0	0
			514	308	103	103			
7	U	103	Total	C	N	O	0	0	0
			514	308	103	103			

- Molecule 8 is SELENIUM ATOM (three-letter code: SE) (formula: Se).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	9	Total	Se	1	0
			9	9		

Continued on next page...

Continued from previous page...

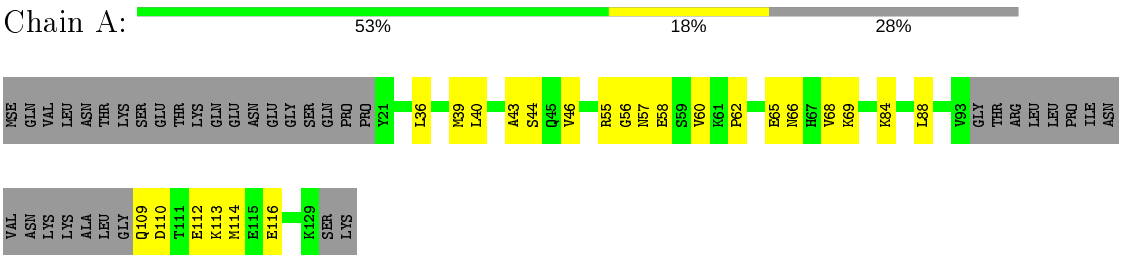
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	5	Total Se 5 5	1	0
8	J	4	Total Se 4 4	3	0
8	Q	4	Total Se 4 4	0	0
8	D	3	Total Se 3 3	0	0
8	K	4	Total Se 4 4	0	0
8	E	6	Total Se 6 6	2	0
8	H	3	Total Se 3 3	2	0
8	B	9	Total Se 9 9	1	0
8	I	10	Total Se 10 10	3	0
8	C	4	Total Se 4 4	1	0
8	A	3	Total Se 3 3	1	0
8	T	2	Total Se 2 2	1	0
8	N	5	Total Se 5 5	1	0
8	U	6	Total Se 6 6	2	0
8	O	3	Total Se 3 3	0	0
8	R	2	Total Se 2 2	0	0
8	L	7	Total Se 7 7	0	0
8	S	6	Total Se 6 6	0	0
8	M	3	Total Se 3 3	3	0

3 Residue-property plots (i)

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 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.

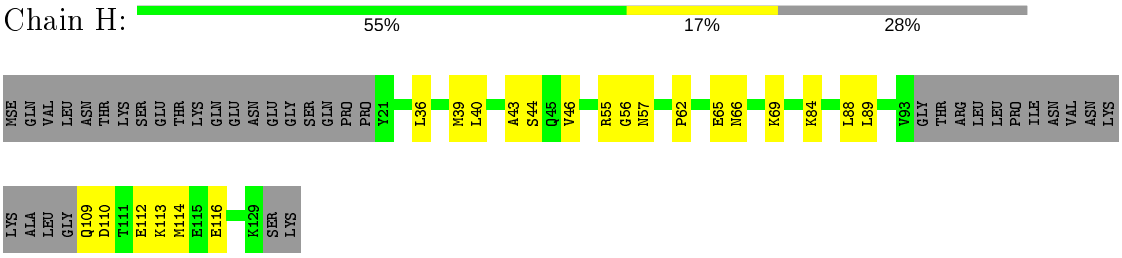
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11

Chain A:



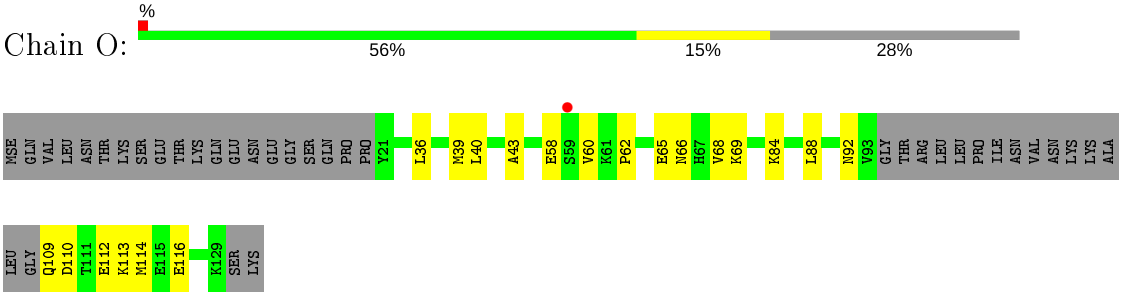
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11

Chain H:



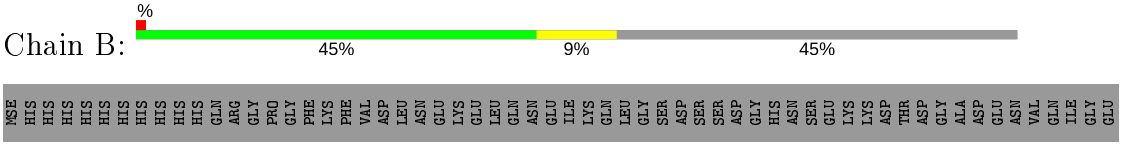
- Molecule 1: Mediator of RNA polymerase II transcription subunit 11

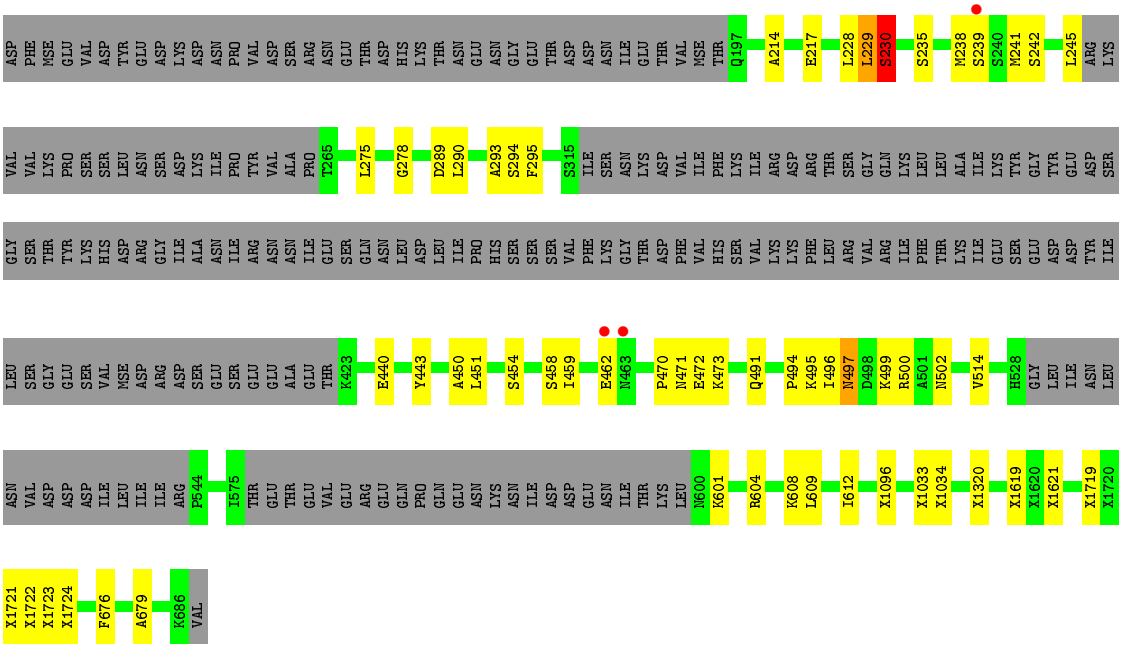
Chain O:



- Molecule 2: Mediator of RNA polymerase II transcription subunit 17

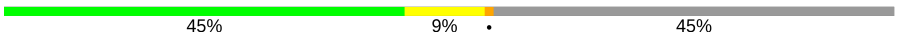
Chain B:

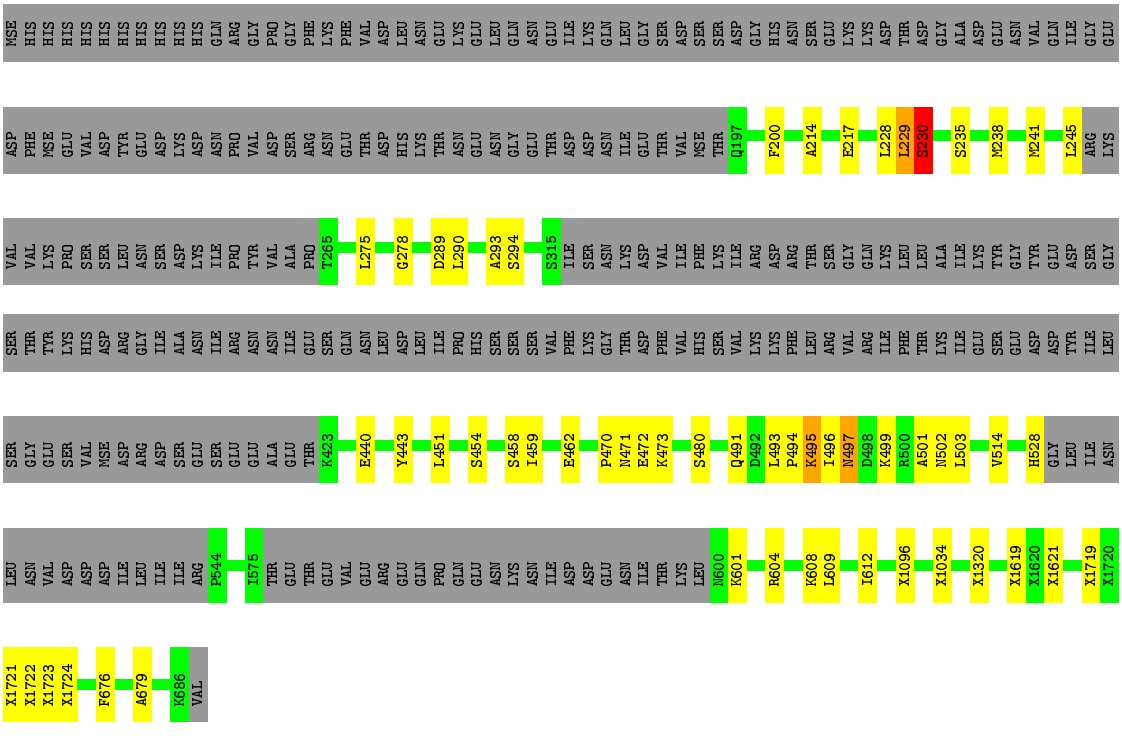




• Molecule 2: Mediator of RNA polymerase II transcription subunit 17

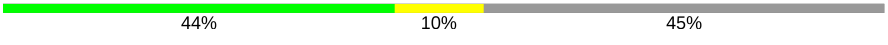
Chain I:

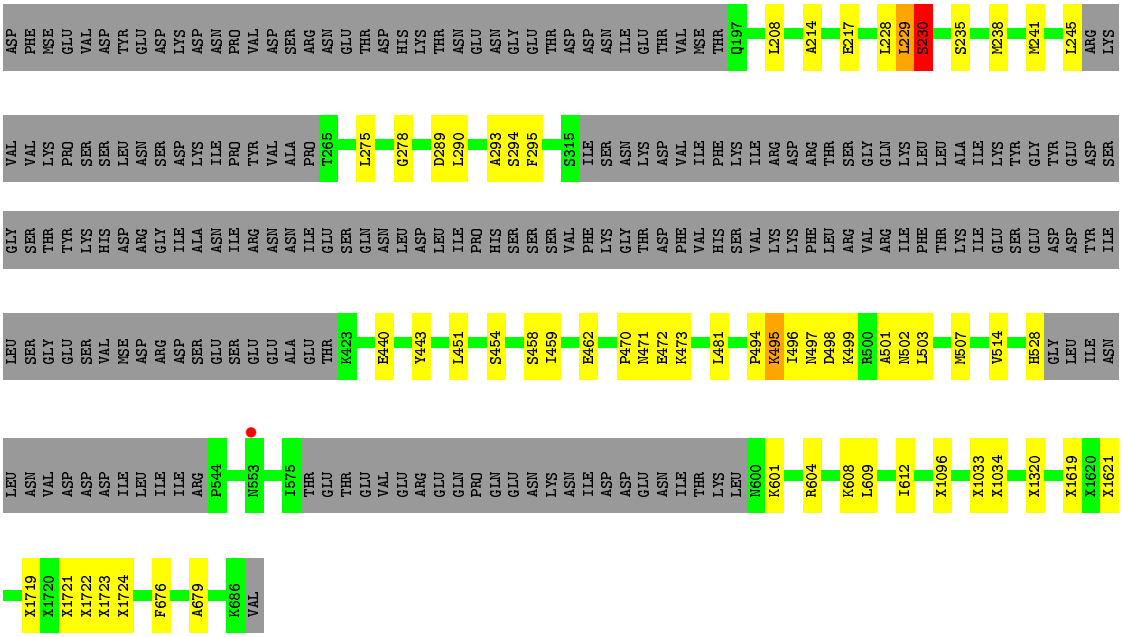




• Molecule 2: Mediator of RNA polymerase II transcription subunit 17

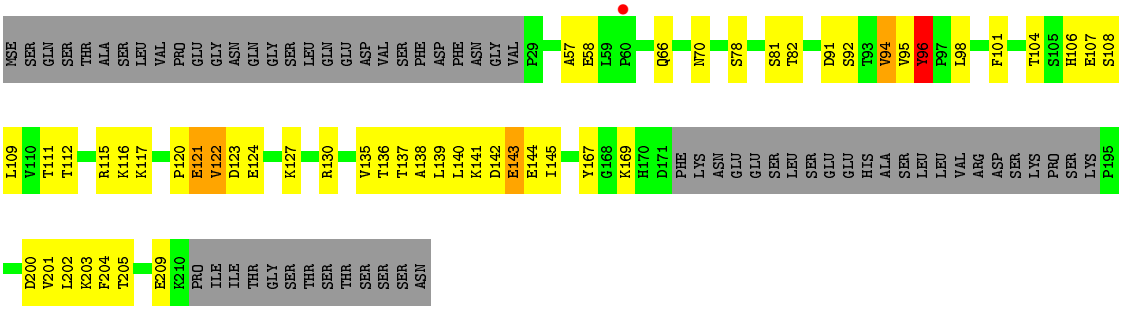
Chain P:





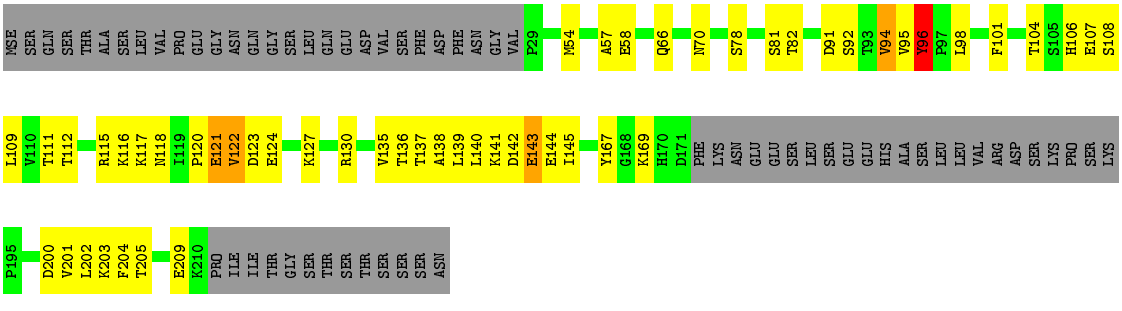
• Molecule 3: Mediator of RNA polymerase II transcription subunit 8

Chain C:



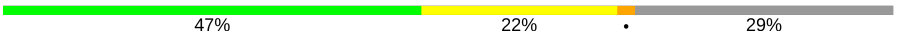
• Molecule 3: Mediator of RNA polymerase II transcription subunit 8

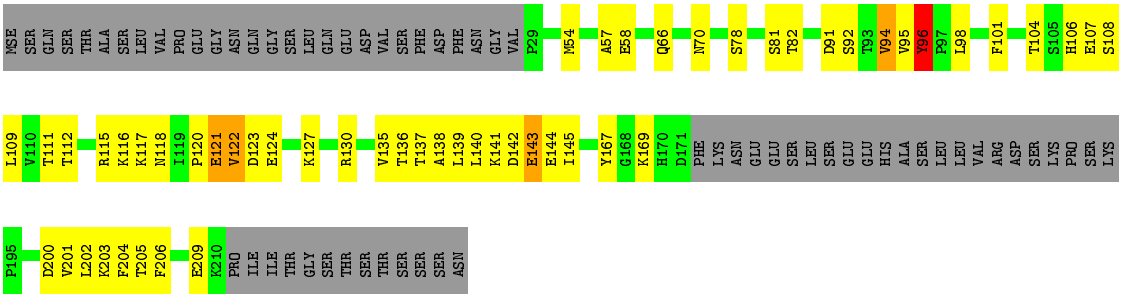
Chain J:



• Molecule 3: Mediator of RNA polymerase II transcription subunit 8

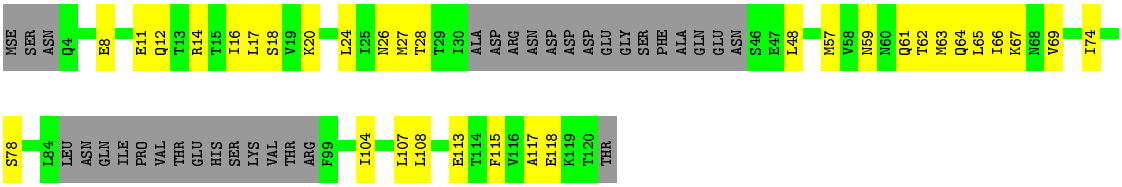
Chain Q:





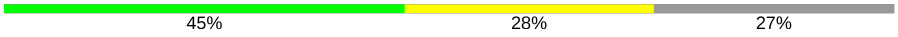
• Molecule 4: Mediator of RNA polymerase II transcription subunit 22

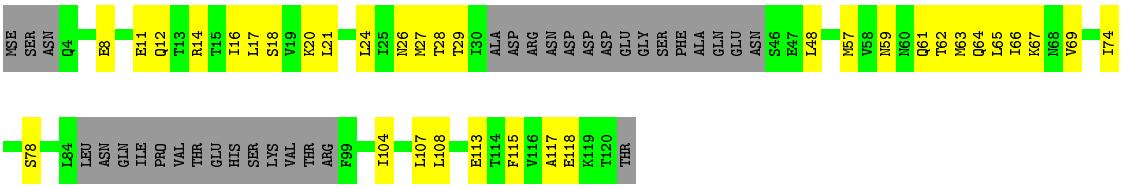
Chain D:



• Molecule 4: Mediator of RNA polymerase II transcription subunit 22

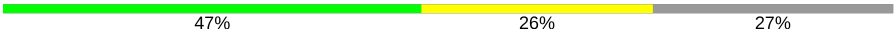
Chain K:

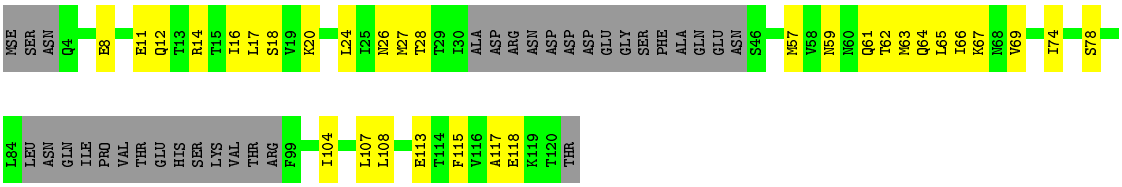




• Molecule 4: Mediator of RNA polymerase II transcription subunit 22

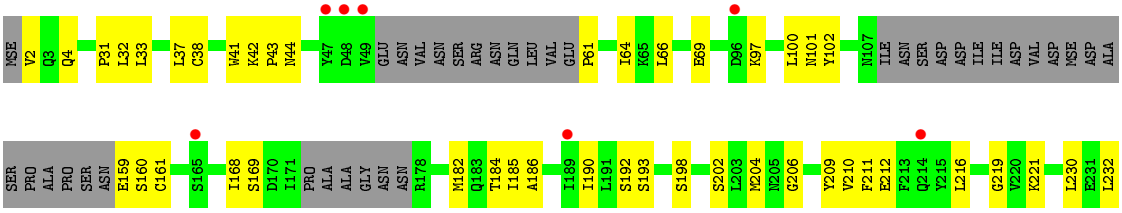
Chain R:

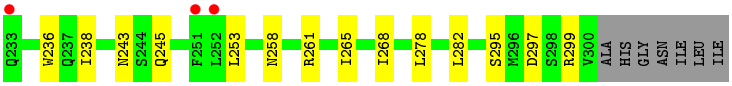




• Molecule 5: Mediator of RNA polymerase II transcription subunit 18

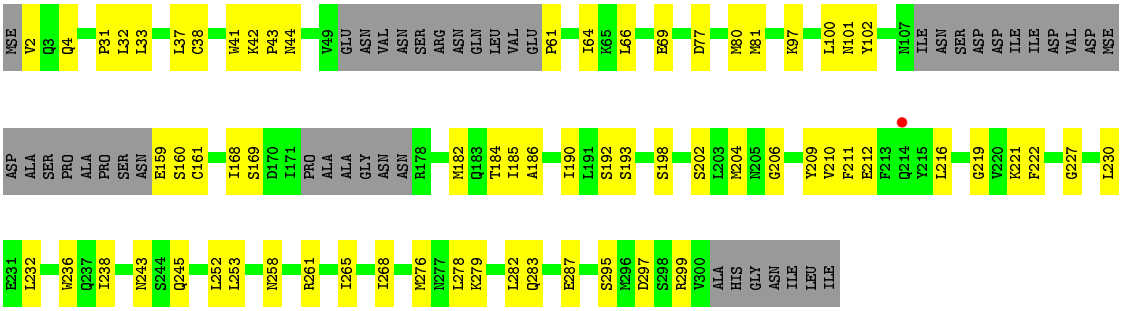
Chain E:





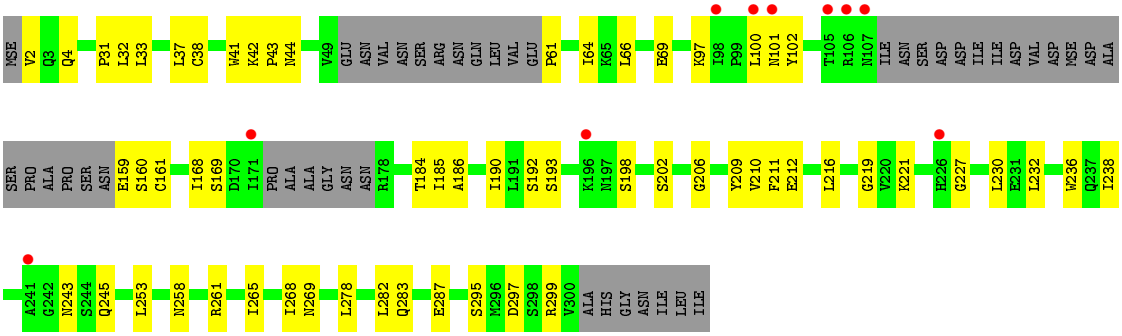
• Molecule 5: Mediator of RNA polymerase II transcription subunit 18

Chain L:



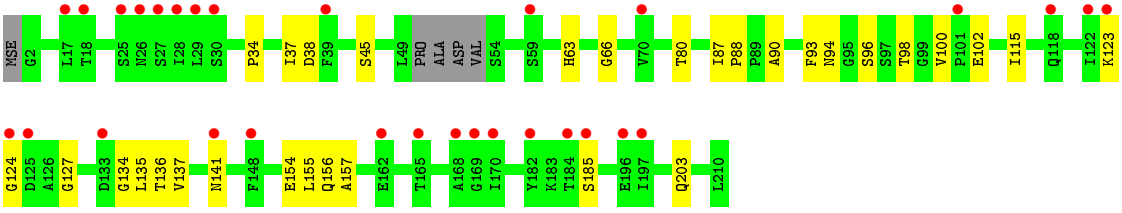
• Molecule 5: Mediator of RNA polymerase II transcription subunit 18

Chain S:



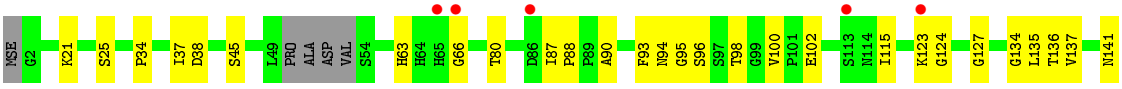
• Molecule 6: Mediator of RNA polymerase II transcription subunit 20

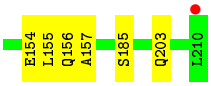
Chain F:



• Molecule 6: Mediator of RNA polymerase II transcription subunit 20

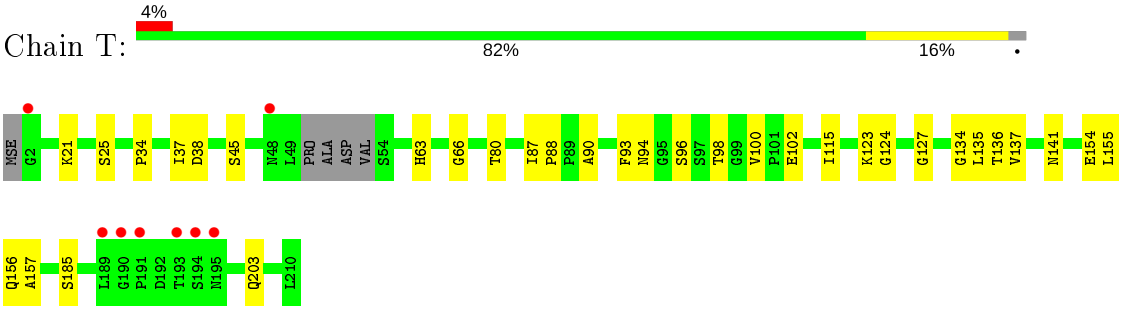
Chain M:





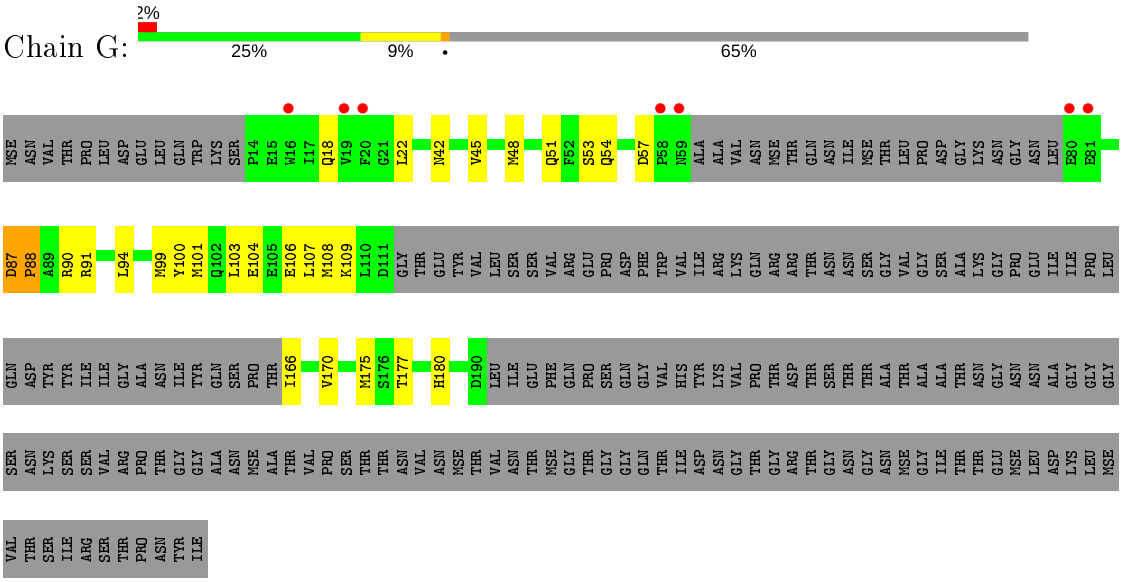
• Molecule 6: Mediator of RNA polymerase II transcription subunit 20

Chain T:



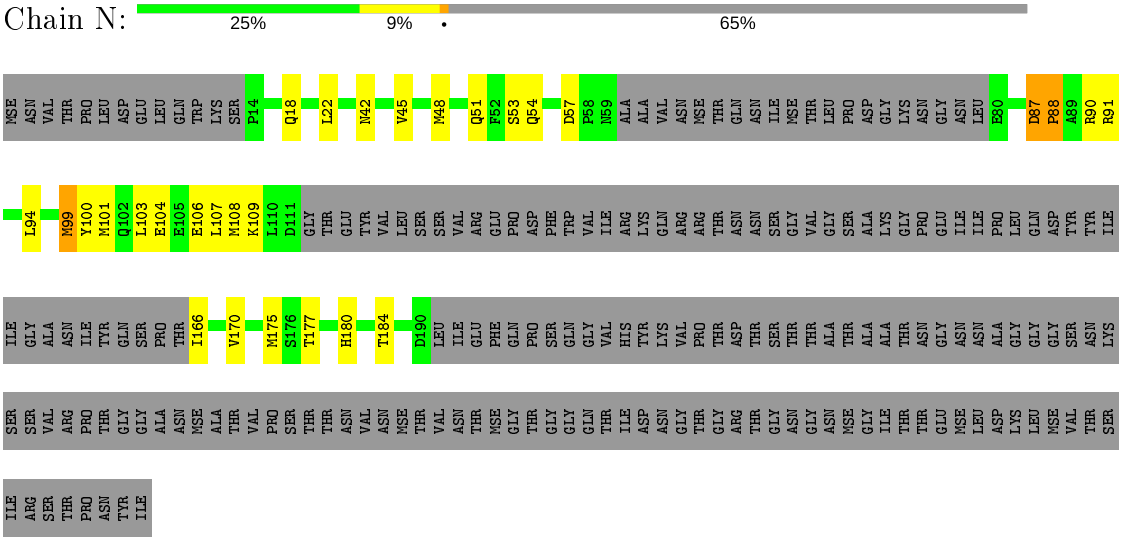
• Molecule 7: Mediator of RNA polymerase II transcription subunit 6

Chain G:



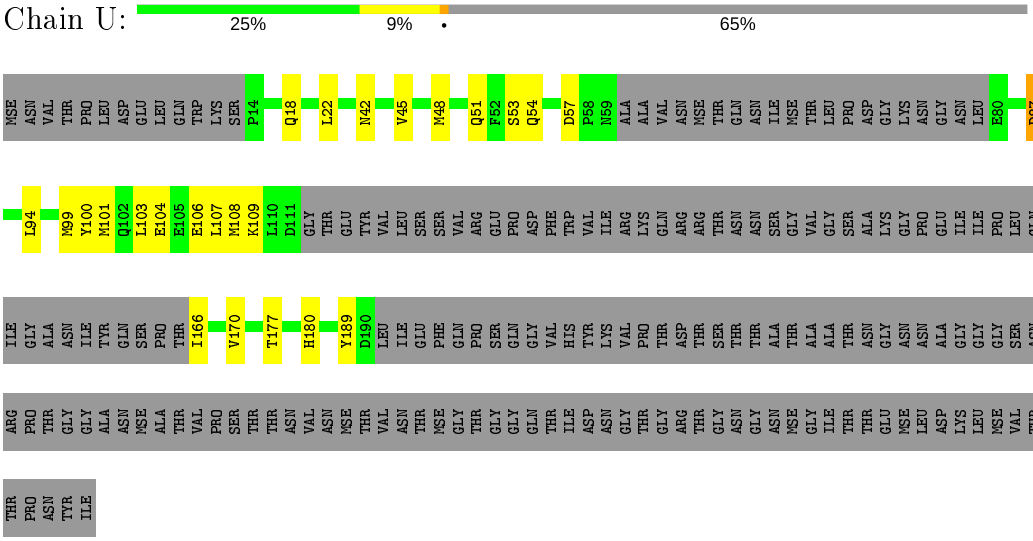
• Molecule 7: Mediator of RNA polymerase II transcription subunit 6

Chain N:



• Molecule 7: Mediator of RNA polymerase II transcription subunit 6

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	265.91Å 265.91Å 319.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.91 – 4.30 49.91 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.91-4.30) 92.6 (49.91-4.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.345 , 0.373 0.344 , 0.342	Depositor DCC
R_{free} test set	4144 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	145.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 467.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.29$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.257 for -h,-k,l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	17945	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: SE

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	0.35	0/464	0.57	0/642
1	H	0.35	0/464	0.57	0/642
1	O	0.35	0/464	0.57	0/642
2	B	0.38	0/1346	0.68	0/1859
2	I	0.38	0/1346	0.70	1/1859 (0.1%)
2	P	0.37	0/1346	0.69	1/1859 (0.1%)
3	C	0.41	0/786	0.75	2/1090 (0.2%)
3	J	0.41	0/786	0.75	2/1090 (0.2%)
3	Q	0.41	0/786	0.75	2/1090 (0.2%)
4	D	0.40	0/433	0.65	0/595
4	K	0.40	0/433	0.65	0/595
4	R	0.40	0/433	0.65	0/595
5	E	0.35	0/1129	0.62	0/1553
5	L	0.35	0/1129	0.62	0/1553
5	S	0.35	0/1129	0.62	0/1553
6	F	0.35	0/1007	0.66	0/1394
6	M	0.35	0/1007	0.65	0/1394
6	T	0.35	0/1007	0.65	0/1394
7	G	0.34	0/506	0.72	1/695 (0.1%)
7	N	0.34	0/506	0.72	1/695 (0.1%)
7	U	0.34	0/506	0.72	1/695 (0.1%)
All	All	0.37	0/17013	0.67	11/23484 (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
2	B	0	2
2	I	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	2
3	C	0	4
3	J	0	4
3	Q	0	4
5	E	0	1
5	L	0	1
5	S	0	1
7	G	0	2
7	N	0	2
7	U	0	2
All	All	0	27

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	98	LEU	C-N-CA	6.54	149.48	122.00
3	J	98	LEU	C-N-CA	6.54	149.46	122.00
3	Q	98	LEU	C-N-CA	6.53	149.41	122.00
2	I	495	LYS	N-CA-C	-5.89	95.10	111.00
3	C	121	GLU	N-CA-C	-5.73	95.53	111.00

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1722	UNK	Peptide
2	B	230	SER	Mainchain
3	C	101	PHE	Peptide
3	C	104	THR	Peptide
3	C	96	TYR	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	468	0	192	17	0
1	H	468	0	192	15	0
1	O	468	0	192	14	0
2	B	1583	0	628	37	0
2	I	1583	0	629	44	0
2	P	1583	0	628	45	0
3	C	791	0	333	52	0
3	J	791	0	333	52	0
3	Q	791	0	333	56	0
4	D	440	0	188	24	0
4	K	440	0	188	31	0
4	R	440	0	188	21	0
5	E	1141	0	481	47	0
5	L	1141	0	481	59	0
5	S	1141	0	481	48	0
6	F	1012	0	469	16	0
6	M	1012	0	469	18	0
6	T	1012	0	469	17	0
7	G	514	0	209	20	0
7	N	514	0	209	24	0
7	U	514	0	209	22	0
8	A	3	0	0	1	0
8	B	9	0	0	4	0
8	C	4	0	0	0	0
8	D	3	0	0	4	0
8	E	6	0	0	6	0
8	G	5	0	0	0	0
8	H	3	0	0	1	0
8	I	10	0	0	4	0
8	J	4	0	0	2	0
8	K	4	0	0	10	0
8	L	7	0	0	14	0
8	M	3	0	0	0	0
8	N	5	0	0	4	0
8	O	3	0	0	3	0
8	P	9	0	0	6	0
8	Q	4	0	0	3	0
8	R	2	0	0	0	0
8	S	6	0	0	2	0
8	T	2	0	0	0	0
8	U	6	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17945	0	7501	642	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 25.

The worst 5 of 642 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)
3:Q:54:MSE:HA	8:Q:325:SE:SE	1.32	1.75
3:Q:54:MSE:CA	8:Q:325:SE:SE	2.29	1.27
4:K:28:THR:HA	8:K:177:SE:SE	1.90	1.22
3:C:143:GLU:O	3:C:145:ILE:N	1.74	1.21
3:J:143:GLU:O	3:J:145:ILE:N	1.74	1.18

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	90/131 (69%)	83 (92%)	7 (8%)	0	100 100
1	H	90/131 (69%)	83 (92%)	7 (8%)	0	100 100
1	O	90/131 (69%)	83 (92%)	7 (8%)	0	100 100
2	B	261/583 (45%)	239 (92%)	16 (6%)	6 (2%)	6 37
2	I	261/583 (45%)	239 (92%)	17 (6%)	5 (2%)	8 41
2	P	261/583 (45%)	241 (92%)	16 (6%)	4 (2%)	10 46
3	C	155/223 (70%)	135 (87%)	14 (9%)	6 (4%)	3 26
3	J	155/223 (70%)	135 (87%)	14 (9%)	6 (4%)	3 26
3	Q	155/223 (70%)	135 (87%)	14 (9%)	6 (4%)	3 26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	82/121 (68%)	69 (84%)	13 (16%)	0	100	100
4	K	82/121 (68%)	69 (84%)	13 (16%)	0	100	100
4	R	82/121 (68%)	69 (84%)	13 (16%)	0	100	100
5	E	223/275 (81%)	193 (86%)	30 (14%)	0	100	100
5	L	223/275 (81%)	193 (86%)	30 (14%)	0	100	100
5	S	223/275 (81%)	193 (86%)	30 (14%)	0	100	100
6	F	201/210 (96%)	185 (92%)	15 (8%)	1 (0%)	29	68
6	M	201/210 (96%)	184 (92%)	16 (8%)	1 (0%)	29	68
6	T	201/210 (96%)	185 (92%)	15 (8%)	1 (0%)	29	68
7	G	97/295 (33%)	82 (84%)	14 (14%)	1 (1%)	15	54
7	N	97/295 (33%)	82 (84%)	14 (14%)	1 (1%)	15	54
7	U	97/295 (33%)	82 (84%)	14 (14%)	1 (1%)	15	54
All	All	3327/5514 (60%)	2959 (89%)	329 (10%)	39 (1%)	13	50

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	230	SER
2	B	497	ASN
2	B	500	ARG
3	C	94	VAL
3	C	144	GLU

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

Of 98 ligands modelled in this entry, 98 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	P	6
2	B	6
2	I	6

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1727:UNK	C	669:GLU	N	41.03
1	I	1727:UNK	C	669:GLU	N	41.03
1	P	1727:UNK	C	669:GLU	N	41.03
1	B	1101:UNK	C	1028:UNK	N	37.71
1	I	1101:UNK	C	1028:UNK	N	37.71

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^{th} 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	92/131 (70%)	-0.83	0 100 100	42, 74, 118, 119	0
1	H	92/131 (70%)	-0.87	0 100 100	29, 42, 119, 121	0
1	O	92/131 (70%)	-0.86	1 (1%) 80 72	80, 92, 168, 169	0
2	B	265/583 (45%)	-0.71	3 (1%) 80 72	32, 87, 179, 181	0
2	I	265/583 (45%)	-0.72	0 100 100	52, 71, 177, 191	0
2	P	265/583 (45%)	-0.75	1 (0%) 92 87	15, 124, 209, 210	0
3	C	156/223 (69%)	-0.73	1 (0%) 89 84	33, 106, 192, 192	0
3	J	156/223 (69%)	-0.72	0 100 100	42, 112, 192, 240	0
3	Q	156/223 (69%)	-0.65	0 100 100	61, 135, 205, 238	0
4	D	84/121 (69%)	-0.85	0 100 100	54, 66, 92, 99	0
4	K	84/121 (69%)	-0.73	0 100 100	54, 59, 113, 114	0
4	R	84/121 (69%)	-0.82	0 100 100	52, 110, 165, 167	0
5	E	223/275 (81%)	-0.20	10 (4%) 33 28	99, 184, 216, 223	0
5	L	223/275 (81%)	-0.52	1 (0%) 92 87	64, 149, 196, 198	0
5	S	223/275 (81%)	-0.22	10 (4%) 33 28	103, 149, 255, 259	0
6	F	202/210 (96%)	0.56	30 (14%) 2 3	187, 252, 349, 353	0
6	M	202/210 (96%)	-0.32	6 (2%) 50 39	96, 134, 194, 199	0
6	T	202/210 (96%)	-0.09	8 (3%) 38 30	40, 182, 243, 247	0
7	G	98/295 (33%)	-0.37	7 (7%) 16 13	33, 147, 171, 172	0
7	N	98/295 (33%)	-0.83	0 100 100	35, 47, 147, 148	0
7	U	98/295 (33%)	-0.66	0 100 100	48, 119, 138, 140	0
All	All	3360/5514 (60%)	-0.51	78 (2%) 60 51	15, 129, 244, 353	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	18	THR	11.4
6	T	194	SER	8.7
6	F	125	ASP	6.4
6	T	48	ASN	6.2
6	F	169	GLY	5.8

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SE	B	904	1/1	0.39	0.78	98,98,98,98	1
8	SE	L	409	1/1	0.40	0.34	98,98,98,98	1
8	SE	I	901	1/1	0.41	0.48	98,98,98,98	1
8	SE	N	397	1/1	0.63	1.97	98,98,98,98	1
8	SE	B	1729	1/1	0.64	0.33	98,98,98,98	1
8	SE	L	412	1/1	0.66	0.71	98,98,98,98	1
8	SE	G	1296	1/1	0.67	1.22	98,98,98,98	1
8	SE	Q	327	1/1	0.76	0.38	98,98,98,98	1
8	SE	D	223	1/1	0.76	1.14	98,98,98,98	1
8	SE	S	311	1/1	0.77	1.21	98,98,98,98	1
8	SE	A	313	1/1	0.84	0.27	98,98,98,98	1
8	SE	R	222	1/1	0.84	0.36	98,98,98,98	1
8	SE	K	177	1/1	0.85	0.19	98,98,98,98	0
8	SE	D	1301	1/1	0.87	0.15	98,98,98,98	0
8	SE	R	223	1/1	0.90	0.40	98,98,98,98	1
8	SE	Q	326	1/1	0.91	0.39	98,98,98,98	1
8	SE	L	408	1/1	0.91	0.20	98,98,98,98	1
8	SE	I	1729	1/1	0.94	0.90	98,98,98,98	1
8	SE	I	906	1/1	0.96	0.16	98,98,98,98	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SE	A	133	1/1	0.96	0.22	98,98,98,98	1
8	SE	D	222	1/1	0.96	0.41	98,98,98,98	0
8	SE	P	1733	1/1	0.97	0.95	98,98,98,98	1
8	SE	N	400	1/1	0.97	0.40	98,98,98,98	0
8	SE	N	398	1/1	0.97	0.10	98,98,98,98	0
8	SE	S	313	1/1	0.97	0.16	98,98,98,98	0
8	SE	J	225	1/1	0.98	0.45	98,98,98,98	1
8	SE	M	313	1/1	-	-	98,98,98,98	1
8	SE	C	224	1/1	0.55	0.19	98,98,98,98	1
8	SE	G	1297	1/1	0.82	0.14	98,98,98,98	1
8	SE	P	1729	1/1	0.86	0.88	98,98,98,98	1
8	SE	U	495	1/1	0.88	0.43	98,98,98,98	0
8	SE	E	413	1/1	-	-	98,98,98,98	1
8	SE	J	224	1/1	-	-	98,98,98,98	1
8	SE	O	133	1/1	0.79	1.30	98,98,98,98	1
8	SE	J	226	1/1	-	-	98,98,98,98	1
8	SE	I	903	1/1	0.83	0.67	98,98,98,98	1
8	SE	B	1728	1/1	0.91	0.11	98,98,98,98	0
8	SE	H	132	1/1	-	-	98,98,98,98	1
8	SE	P	1732	1/1	-	-	98,98,98,98	1
8	SE	U	500	1/1	0.88	0.70	98,98,98,98	1
8	SE	K	175	1/1	0.93	0.24	98,98,98,98	1
8	SE	N	399	1/1	-	-	98,98,98,98	1
8	SE	P	902	1/1	0.91	0.70	98,98,98,98	1
8	SE	H	133	1/1	-	-	98,98,98,98	1
8	SE	E	409	1/1	0.94	0.12	98,98,98,98	1
8	SE	T	312	1/1	-	-	98,98,98,98	1
8	SE	U	498	1/1	-	-	98,98,98,98	1
8	SE	I	1728	1/1	0.84	0.78	98,98,98,98	1
8	SE	E	408	1/1	-	-	98,98,98,98	1
8	SE	B	1731	1/1	-	-	98,98,98,98	1
8	SE	U	499	1/1	0.95	0.06	98,98,98,98	1
8	SE	I	902	1/1	-	-	98,98,98,98	1
8	SE	I	904	1/1	-0.04	1.53	98,98,98,98	1
8	SE	L	414	1/1	0.64	2.61	98,98,98,98	1
8	SE	T	311	1/1	0.76	0.20	98,98,98,98	1
8	SE	B	902	1/1	0.80	0.22	98,98,98,98	1
8	SE	I	905	1/1	0.97	0.07	98,98,98,98	0
8	SE	G	1299	1/1	0.98	0.14	98,98,98,98	1
8	SE	N	396	1/1	0.98	0.27	98,98,98,98	1
8	SE	I	1731	1/1	-	-	98,98,98,98	1
8	SE	L	413	1/1	0.82	0.10	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SE	P	901	1/1	0.85	0.99	98,98,98,98	1
8	SE	K	173	1/1	0.87	1.14	98,98,98,98	1
8	SE	B	1730	1/1	0.96	0.20	98,98,98,98	1
8	SE	I	1730	1/1	-	-	98,98,98,98	1
8	SE	P	1730	1/1	0.75	0.32	98,98,98,98	0
8	SE	Q	324	1/1	0.87	0.38	98,98,98,98	1
8	SE	K	174	1/1	0.92	0.17	98,98,98,98	1
8	SE	S	308	1/1	0.93	0.41	98,98,98,98	1
8	SE	L	410	1/1	0.93	0.15	98,98,98,98	0
8	SE	C	226	1/1	0.94	1.56	98,98,98,98	1
8	SE	B	901	1/1	0.99	0.09	98,98,98,98	0
8	SE	A	132	1/1	-	-	98,98,98,98	1
8	SE	S	309	1/1	0.60	1.32	98,98,98,98	1
8	SE	P	900	1/1	0.81	0.64	98,98,98,98	1
8	SE	E	412	1/1	0.91	0.14	98,98,98,98	1
8	SE	E	411	1/1	0.91	0.12	98,98,98,98	0
8	SE	Q	325	1/1	0.95	0.50	98,98,98,98	1
8	SE	U	496	1/1	0.96	0.45	98,98,98,98	1
8	SE	M	311	1/1	-	-	98,98,98,98	1
8	SE	U	497	1/1	-	-	98,98,98,98	1
8	SE	S	312	1/1	0.23	1.43	98,98,98,98	1
8	SE	J	227	1/1	-	-	98,98,98,98	1
8	SE	M	312	1/1	-	-	98,98,98,98	1
8	SE	C	225	1/1	0.75	0.51	98,98,98,98	1
8	SE	P	1731	1/1	0.79	0.95	98,98,98,98	1
8	SE	P	1728	1/1	0.81	0.35	98,98,98,98	1
8	SE	B	1732	1/1	0.85	0.56	98,98,98,98	1
8	SE	B	903	1/1	0.86	0.29	98,98,98,98	1
8	SE	L	415	1/1	0.91	1.16	98,98,98,98	1
8	SE	E	410	1/1	0.94	0.51	98,98,98,98	1
8	SE	O	132	1/1	0.96	0.12	98,98,98,98	1
8	SE	C	227	1/1	-	-	98,98,98,98	1
8	SE	G	1298	1/1	-	-	98,98,98,98	1
8	SE	H	313	1/1	0.65	0.59	98,98,98,98	1
8	SE	O	313	1/1	0.93	0.06	98,98,98,98	0
8	SE	S	310	1/1	0.95	0.07	98,98,98,98	0
8	SE	G	1300	1/1	0.97	0.55	98,98,98,98	0

6.5 Other polymers

There are no such residues in this entry.