



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:45 PM UTC

PDB ID : 6XWX / pdb_00006xwx
Title : Crystal structure of the Tof1-Csm3 complex
Authors : Grabarczyk, D.B.
Deposited on : 2020-01-24
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

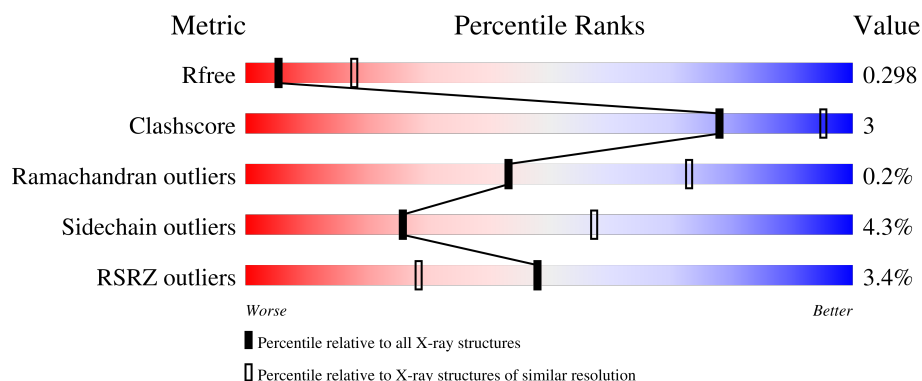
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	599	3% 80% 13% 6%
1	C	599	3% 83% 10% 6%
1	E	599	4% 84% 10% 6%
2	B	111	2% 60% 14% 24%
2	D	111	3% 65% 9% 26%

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Mol	Chain	Length	Quality of chain
2	F	111	5% 56% 8% 36%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15731 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 Uncharacterized protein,Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	0	0
			4580	2933	789	837	21			
1	C	562	Total	C	N	O	S	0	0	0
			4579	2930	788	840	21			
1	E	566	Total	C	N	O	S	0	0	0
			4623	2964	792	845	22			

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP G0S825
A	-17	LYS	-	expression tag	UNP G0S825
A	-16	HIS	-	expression tag	UNP G0S825
A	-15	HIS	-	expression tag	UNP G0S825
A	-14	HIS	-	expression tag	UNP G0S825
A	-13	HIS	-	expression tag	UNP G0S825
A	-12	HIS	-	expression tag	UNP G0S825
A	-11	HIS	-	expression tag	UNP G0S825
A	-10	SER	-	expression tag	UNP G0S825
A	-9	ALA	-	expression tag	UNP G0S825
A	-8	GLY	-	expression tag	UNP G0S825
A	-7	LEU	-	expression tag	UNP G0S825
A	-6	GLU	-	expression tag	UNP G0S825
A	-5	VAL	-	expression tag	UNP G0S825
A	-4	LEU	-	expression tag	UNP G0S825
A	-3	PHE	-	expression tag	UNP G0S825
A	-2	GLN	-	expression tag	UNP G0S825
A	-1	GLY	-	expression tag	UNP G0S825
A	0	PRO	-	expression tag	UNP G0S825
A	257	GLY	-	linker	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	SER	deletion	UNP G0S825
A	?	-	SER	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	GLN	deletion	UNP G0S825
A	?	-	SER	deletion	UNP G0S825
A	?	-	GLY	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	VAL	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	ARG	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	LYS	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	ALA	deletion	UNP G0S825
A	?	-	GLY	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASN	deletion	UNP G0S825
A	?	-	GLY	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	GLN	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	GLU	deletion	UNP G0S825
A	?	-	ASP	deletion	UNP G0S825
A	437	GLY	ASP	conflict	UNP G0S825
C	-18	MET	-	initiating methionine	UNP G0S825
C	-17	LYS	-	expression tag	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP G0S825
C	-15	HIS	-	expression tag	UNP G0S825
C	-14	HIS	-	expression tag	UNP G0S825
C	-13	HIS	-	expression tag	UNP G0S825
C	-12	HIS	-	expression tag	UNP G0S825
C	-11	HIS	-	expression tag	UNP G0S825
C	-10	SER	-	expression tag	UNP G0S825
C	-9	ALA	-	expression tag	UNP G0S825
C	-8	GLY	-	expression tag	UNP G0S825
C	-7	LEU	-	expression tag	UNP G0S825
C	-6	GLU	-	expression tag	UNP G0S825
C	-5	VAL	-	expression tag	UNP G0S825
C	-4	LEU	-	expression tag	UNP G0S825
C	-3	PHE	-	expression tag	UNP G0S825
C	-2	GLN	-	expression tag	UNP G0S825
C	-1	GLY	-	expression tag	UNP G0S825
C	0	PRO	-	expression tag	UNP G0S825
C	257	GLY	-	linker	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	SER	deletion	UNP G0S825
C	?	-	SER	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	GLN	deletion	UNP G0S825
C	?	-	SER	deletion	UNP G0S825
C	?	-	GLY	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	VAL	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	ARG	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	LYS	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	ALA	deletion	UNP G0S825
C	?	-	GLY	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASN	deletion	UNP G0S825
C	?	-	GLY	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	GLN	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	GLU	deletion	UNP G0S825
C	?	-	ASP	deletion	UNP G0S825
C	437	GLY	ASP	conflict	UNP G0S825
E	-18	MET	-	initiating methionine	UNP G0S825
E	-17	LYS	-	expression tag	UNP G0S825
E	-16	HIS	-	expression tag	UNP G0S825
E	-15	HIS	-	expression tag	UNP G0S825
E	-14	HIS	-	expression tag	UNP G0S825
E	-13	HIS	-	expression tag	UNP G0S825
E	-12	HIS	-	expression tag	UNP G0S825
E	-11	HIS	-	expression tag	UNP G0S825
E	-10	SER	-	expression tag	UNP G0S825
E	-9	ALA	-	expression tag	UNP G0S825
E	-8	GLY	-	expression tag	UNP G0S825
E	-7	LEU	-	expression tag	UNP G0S825
E	-6	GLU	-	expression tag	UNP G0S825
E	-5	VAL	-	expression tag	UNP G0S825
E	-4	LEU	-	expression tag	UNP G0S825
E	-3	PHE	-	expression tag	UNP G0S825
E	-2	GLN	-	expression tag	UNP G0S825
E	-1	GLY	-	expression tag	UNP G0S825
E	0	PRO	-	expression tag	UNP G0S825
E	257	GLY	-	linker	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LYS	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	SER	deletion	UNP G0S825
E	?	-	SER	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	GLN	deletion	UNP G0S825
E	?	-	SER	deletion	UNP G0S825
E	?	-	GLY	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	VAL	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	ARG	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	LYS	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	ALA	deletion	UNP G0S825
E	?	-	GLY	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASN	deletion	UNP G0S825
E	?	-	GLY	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	GLN	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	GLU	deletion	UNP G0S825
E	?	-	ASP	deletion	UNP G0S825
E	437	GLY	ASP	conflict	UNP G0S825

- Molecule 2 is a protein called Chromosome segregation in meiosis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	0	0
			693	447	125	119	2			
2	D	82	Total	C	N	O	S	0	0	0
			675	436	120	117	2			
2	F	71	Total	C	N	O	S	0	0	0
			581	378	104	97	2			

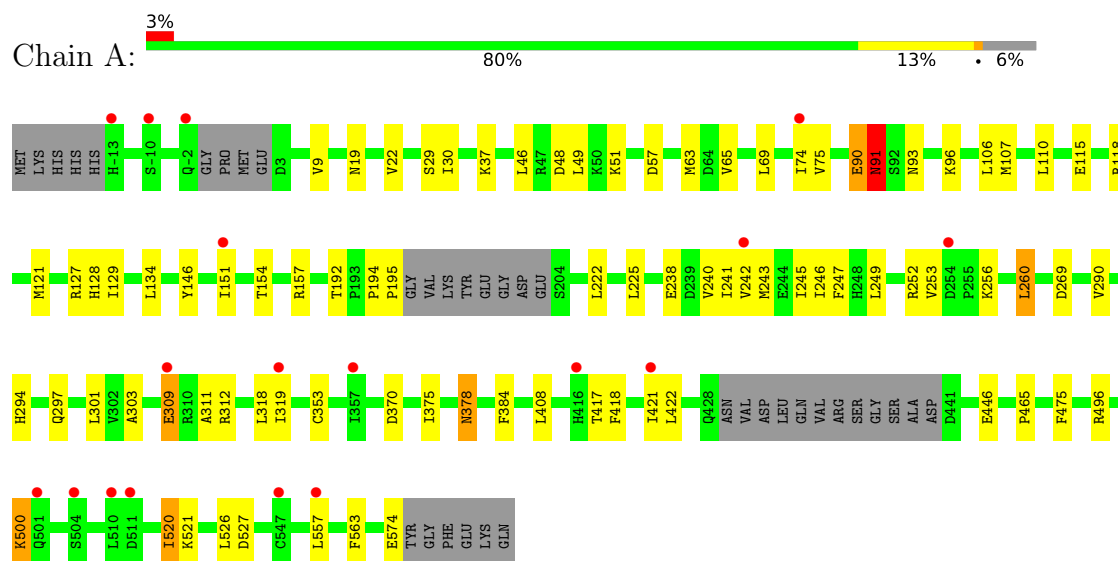
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	MET	-	initiating methionine	UNP G0S0S7
D	47	MET	-	initiating methionine	UNP G0S0S7
F	47	MET	-	initiating methionine	UNP G0S0S7

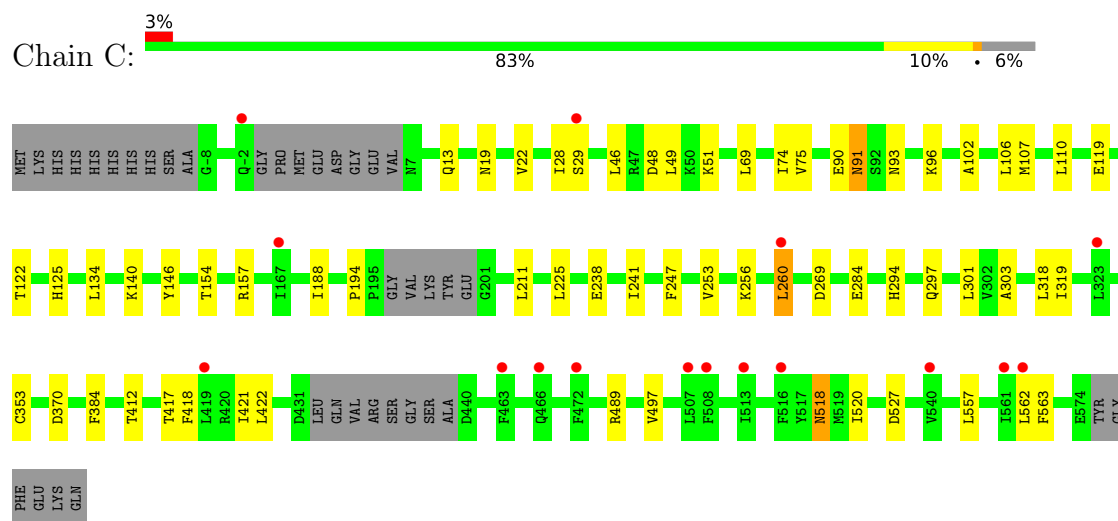
3 Residue-property plots [i](#)

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.

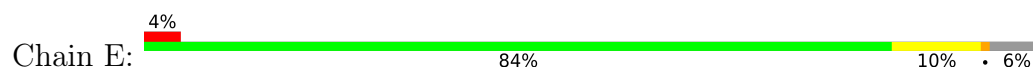
- Molecule 1: Uncharacterized protein,Uncharacterized protein

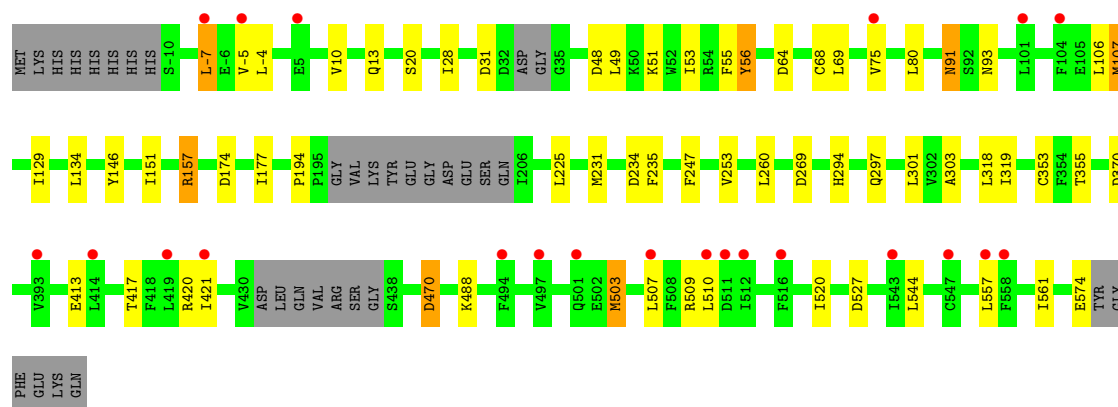


- Molecule 1: Uncharacterized protein,Uncharacterized protein

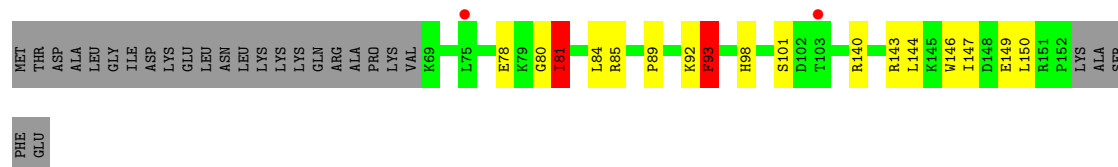


- Molecule 1: Uncharacterized protein,Uncharacterized protein

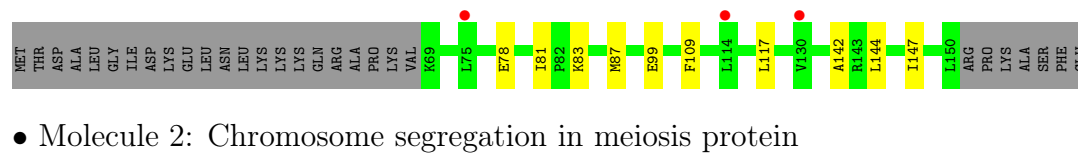




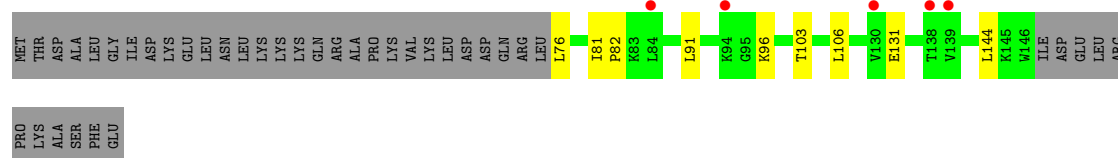
- Molecule 2: Chromosome segregation in meiosis protein



- Molecule 2: Chromosome segregation in meiosis protein



- Molecule 2: Chromosome segregation in meiosis protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.47Å 82.03Å 161.16Å 90.00° 124.85° 90.00°	Depositor
Resolution (Å)	45.73 – 3.10 45.73 – 3.10	Depositor EDS
% Data completeness (in resolution range)	52.3 (45.73-3.10) 52.3 (45.73-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.237 , 0.264 0.262 , 0.298	Depositor DCC
R_{free} test set	1355 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	93.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15731	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.75	2/4677 (0.0%)	1.40	13/6322 (0.2%)
1	C	0.75	0/4676	1.40	6/6320 (0.1%)
1	E	0.75	1/4722 (0.0%)	1.41	14/6382 (0.2%)
2	B	0.70	0/708	1.41	6/948 (0.6%)
2	D	0.71	0/689	1.33	2/922 (0.2%)
2	F	0.72	0/595	1.27	0/796
All	All	0.75	3/16067 (0.0%)	1.40	41/21690 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	ILE	CA-CB	5.52	1.56	1.54
1	A	151	ILE	CG1-CD1	-5.32	1.31	1.51
1	A	129	ILE	CA-CB	5.29	1.56	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	ILE	N-CA-CB	7.71	115.36	110.50
1	A	563	PHE	CA-CB-CG	7.34	121.14	113.80
1	A	309	GLU	CB-CG-CD	7.32	125.04	112.60
2	B	80	GLY	CA-C-N	6.72	124.47	120.24
2	B	80	GLY	C-N-CA	6.72	124.47	120.24
1	A	312	ARG	CA-C-N	6.55	131.70	122.46
1	A	312	ARG	C-N-CA	6.55	131.70	122.46
1	E	470	ASP	CA-CB-CG	6.54	119.14	112.60
1	E	93	ASN	CA-CB-CG	6.46	119.06	112.60
1	E	91	ASN	CA-CB-CG	6.36	118.96	112.60
1	C	91	ASN	CA-CB-CG	6.35	118.95	112.60
1	E	56	TYR	CA-C-N	6.23	128.92	120.38
1	E	56	TYR	C-N-CA	6.23	128.92	120.38
1	A	465	PRO	CA-C-N	6.08	128.71	120.38
1	A	465	PRO	C-N-CA	6.08	128.71	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	LYS	N-CA-C	-5.91	105.66	114.64
2	B	93	PHE	CA-CB-CG	5.86	119.66	113.80
1	A	146	TYR	CA-C-N	5.64	127.84	120.28
1	A	146	TYR	C-N-CA	5.64	127.84	120.28
1	E	488	LYS	CA-C-N	5.62	128.13	120.54
1	E	488	LYS	C-N-CA	5.62	128.13	120.54
1	C	146	TYR	CA-C-N	5.62	127.81	120.28
1	C	146	TYR	C-N-CA	5.62	127.81	120.28
1	E	-7	LEU	CA-C-N	5.61	128.06	120.38
1	E	-7	LEU	C-N-CA	5.61	128.06	120.38
2	B	89	PRO	CA-C-N	5.50	127.66	120.28
2	B	89	PRO	C-N-CA	5.50	127.66	120.28
1	C	563	PHE	CA-CB-CG	5.48	119.28	113.80
1	E	146	TYR	CA-C-N	5.43	127.56	120.28
1	E	146	TYR	C-N-CA	5.43	127.56	120.28
1	E	194	PRO	N-CA-C	5.42	117.31	110.70
1	A	128	HIS	CA-C-N	5.38	125.60	120.43
1	A	128	HIS	C-N-CA	5.38	125.60	120.43
1	A	378	ASN	CA-CB-CG	5.35	117.95	112.60
1	C	194	PRO	N-CA-C	5.22	117.06	110.70
1	E	107	MET	CA-C-N	5.19	124.48	120.33
1	E	107	MET	C-N-CA	5.19	124.48	120.33
1	A	91	ASN	CA-CB-CG	5.19	117.79	112.60
1	C	518	ASN	CA-CB-CG	5.12	117.72	112.60
2	D	142	ALA	CA-C-N	5.00	127.39	120.29
2	D	142	ALA	C-N-CA	5.00	127.39	120.29

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	4580	0	4534	35	0
1	C	4579	0	4535	22	0
1	E	4623	0	4607	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	693	0	720	5	0
2	D	675	0	700	3	0
2	F	581	0	604	3	0
All	All	15731	0	15700	88	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 3.

All (88) 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:9:VAL:HG11	1:A:127:ARG:HE	1.49	0.76
1:E:10:VAL:HG11	1:E:68:CYS:SG	2.35	0.67
1:E:91:ASN:HB3	1:E:157:ARG:HH11	1.65	0.61
1:C:238:GLU:HA	1:C:241:ILE:HD12	1.82	0.61
1:C:19:ASN:HA	1:C:22:VAL:HG22	1.83	0.61
1:A:19:ASN:HA	1:A:22:VAL:HG22	1.83	0.61
1:A:93:ASN:HB3	1:A:96:LYS:HB2	1.83	0.60
1:C:93:ASN:HB3	1:C:96:LYS:HB2	1.84	0.60
1:E:247:PHE:HB2	1:E:301:LEU:HD11	1.83	0.60
1:C:91:ASN:HB3	1:C:157:ARG:HH21	1.68	0.59
1:A:247:PHE:HB2	1:A:301:LEU:HD11	1.85	0.59
1:A:238:GLU:HA	1:A:241:ILE:HD12	1.83	0.58
1:E:503:MET:HE2	1:E:574:GLU:HA	1.83	0.58
2:B:98:HIS:CD2	2:B:101:SER:H	2.22	0.58
1:A:91:ASN:HB2	1:A:157:ARG:HH11	1.69	0.57
1:A:192:THR:HG21	1:A:252:ARG:HH22	1.70	0.56
1:C:75:VAL:HG13	1:C:107:MET:HG2	1.89	0.55
1:E:174:ASP:HA	1:E:177:ILE:HD12	1.91	0.53
1:E:355:THR:HG21	1:E:413:GLU:HG2	1.91	0.53
1:C:303:ALA:HB2	1:C:353:CYS:HA	1.90	0.53
1:C:28:ILE:HG13	1:C:29:SER:H	1.73	0.53
1:A:118:ARG:HD2	1:A:121:MET:HE3	1.91	0.52
1:A:303:ALA:HB2	1:A:353:CYS:HA	1.92	0.51
1:E:75:VAL:HG13	1:E:107:MET:HG2	1.93	0.51
2:D:87:MET:HB3	2:D:109:PHE:HZ	1.76	0.50
2:B:85:ARG:HB3	2:B:146:TRP:HE1	1.76	0.50
1:C:253:VAL:HG21	1:C:260:LEU:HD21	1.93	0.50
1:E:303:ALA:HB2	1:E:353:CYS:HA	1.93	0.50
1:C:269:ASP:HA	1:C:318:LEU:HD22	1.94	0.49
1:C:294:HIS:HA	1:C:297:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:LEU:HB3	2:F:103:THR:HG21	1.93	0.49
1:E:269:ASP:HA	1:E:318:LEU:HD22	1.94	0.49
2:B:93:PHE:HD1	2:B:93:PHE:H	1.61	0.48
1:A:75:VAL:HG13	1:A:107:MET:HG2	1.95	0.48
1:A:57:ASP:CG	1:A:65:VAL:HG22	2.39	0.48
1:A:242:VAL:HA	1:A:245:ILE:HD12	1.96	0.48
1:A:269:ASP:HA	1:A:318:LEU:HD22	1.95	0.47
1:C:412:THR:HG22	1:C:489:ARG:HE	1.80	0.46
1:A:154:THR:HA	1:A:157:ARG:HD3	1.97	0.46
2:D:83:LYS:HG3	2:D:87:MET:HE2	1.97	0.46
2:F:81:ILE:HG13	2:F:82:PRO:HD3	1.98	0.46
1:A:49:LEU:HD22	1:A:69:LEU:HD21	1.98	0.45
1:A:118:ARG:HB2	1:A:121:MET:HG2	1.99	0.45
1:C:154:THR:HA	1:C:157:ARG:HD3	1.97	0.45
1:A:496:ARG:O	1:A:500:LYS:HB2	2.17	0.45
1:E:294:HIS:HA	1:E:297:GLN:HE21	1.81	0.45
1:E:503:MET:HG2	1:E:574:GLU:HG3	1.99	0.45
1:A:408:LEU:HD21	1:A:475:PHE:HA	1.99	0.45
1:A:240:VAL:HG11	1:A:290:VAL:HG12	1.98	0.44
1:A:294:HIS:HA	1:A:297:GLN:HE21	1.81	0.44
1:E:48:ASP:HA	1:E:51:LYS:HD3	1.99	0.44
1:C:140:LYS:HE3	1:C:211:LEU:HD13	1.98	0.44
1:C:384:PHE:HD1	1:C:422:LEU:HD22	1.83	0.44
1:A:520:ILE:HG22	1:A:521:LYS:HG3	1.98	0.44
1:C:49:LEU:HD22	1:C:69:LEU:HD21	1.99	0.44
1:E:417:THR:HG22	1:E:420:ARG:HH21	1.81	0.43
1:A:417:THR:O	1:A:421:ILE:HG12	2.18	0.43
1:A:384:PHE:HD1	1:A:422:LEU:HD22	1.84	0.43
1:A:48:ASP:HA	1:A:51:LYS:HD3	1.99	0.43
1:C:247:PHE:HB2	1:C:301:LEU:HD11	2.00	0.43
1:A:246:ILE:HA	1:A:249:LEU:HD12	2.00	0.43
1:C:417:THR:O	1:C:421:ILE:HG12	2.18	0.43
1:C:48:ASP:HA	1:C:51:LYS:HD3	2.00	0.43
1:E:510:LEU:HG	1:E:561:ILE:HG12	2.01	0.43
1:E:49:LEU:HD22	1:E:69:LEU:HD21	2.01	0.43
1:A:90:GLU:HG2	1:A:96:LYS:HD2	2.01	0.42
1:E:-7:LEU:HB3	1:E:-4:LEU:HD12	2.01	0.42
1:C:19:ASN:HB2	1:E:55:PHE:HB3	2.01	0.42
1:C:119:GLU:HA	1:C:125:HIS:HB3	2.00	0.42
2:D:78:GLU:HG2	2:D:81:ILE:HB	2.01	0.42
1:A:256:LYS:HG2	1:A:311:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PRO:HA	1:A:195:PRO:HD3	1.97	0.42
1:A:29:SER:HA	1:A:37:LYS:HE2	2.02	0.41
1:A:375:ILE:HD13	1:A:378:ASN:HD21	1.84	0.41
1:C:46:LEU:HB3	1:C:102:ALA:HB1	2.02	0.41
2:B:81:ILE:HA	2:B:84:LEU:HD12	2.02	0.41
1:E:253:VAL:HG11	1:E:260:LEU:HD13	2.03	0.41
1:A:69:LEU:HD13	1:A:110:LEU:HD11	2.03	0.41
1:A:526:LEU:HG	1:A:526:LEU:O	2.21	0.41
2:B:140:ARG:HD2	2:B:143:ARG:HH21	1.86	0.41
1:A:115:GLU:HB2	1:A:118:ARG:HE	1.86	0.41
1:A:253:VAL:HG11	1:A:260:LEU:HD21	2.03	0.40
1:E:56:TYR:HE2	1:E:64:ASP:HB2	1.86	0.40
1:E:509:ARG:HH12	2:F:131:GLU:HB2	1.85	0.40
1:A:243:MET:HG2	1:A:301:LEU:HD13	2.04	0.40
1:C:69:LEU:HD13	1:C:110:LEU:HD11	2.04	0.40
1:E:80:LEU:HD22	1:E:151:ILE:HG13	2.03	0.40
1:E:231:MET:HA	1:E:235:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	556/599 (93%)	533 (96%)	22 (4%)	1 (0%)	43	73
1	C	554/599 (92%)	534 (96%)	19 (3%)	1 (0%)	43	73
1	E	558/599 (93%)	532 (95%)	24 (4%)	2 (0%)	30	61
2	B	82/111 (74%)	80 (98%)	2 (2%)	0	100	100
2	D	80/111 (72%)	78 (98%)	2 (2%)	0	100	100
2	F	69/111 (62%)	64 (93%)	5 (7%)	0	100	100
All	All	1899/2130 (89%)	1821 (96%)	74 (4%)	4 (0%)	43	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	503	MET
1	A	527	ASP
1	C	527	ASP
1	E	527	ASP

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	489/528 (93%)	470 (96%)	19 (4%)	28	60
1	C	492/528 (93%)	473 (96%)	19 (4%)	28	60
1	E	500/528 (95%)	482 (96%)	18 (4%)	31	62
2	B	73/96 (76%)	65 (89%)	8 (11%)	6	24
2	D	71/96 (74%)	67 (94%)	4 (6%)	19	49
2	F	60/96 (62%)	55 (92%)	5 (8%)	10	35
All	All	1685/1872 (90%)	1612 (96%)	73 (4%)	26	57

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	46	LEU
1	A	63	MET
1	A	74	ILE
1	A	90	GLU
1	A	91	ASN
1	A	106	LEU
1	A	134	LEU
1	A	222	LEU
1	A	225	LEU
1	A	260	LEU
1	A	309	GLU
1	A	319	ILE

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Mol	Chain	Res	Type
1	A	370	ASP
1	A	418	PHE
1	A	446	GLU
1	A	520	ILE
1	A	557	LEU
1	A	574	GLU
2	B	78	GLU
2	B	81	ILE
2	B	92	LYS
2	B	93	PHE
2	B	144	LEU
2	B	147	ILE
2	B	149	GLU
2	B	150	LEU
1	C	13	GLN
1	C	74	ILE
1	C	90	GLU
1	C	106	LEU
1	C	122	THR
1	C	134	LEU
1	C	188	ILE
1	C	225	LEU
1	C	256	LYS
1	C	260	LEU
1	C	284	GLU
1	C	319	ILE
1	C	370	ASP
1	C	418	PHE
1	C	497	VAL
1	C	518	ASN
1	C	520	ILE
1	C	557	LEU
1	C	562	LEU
2	D	99	GLU
2	D	117	LEU
2	D	144	LEU
2	D	147	ILE
1	E	-5	VAL
1	E	13	GLN
1	E	20	SER
1	E	28	ILE
1	E	31	ASP

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Mol	Chain	Res	Type
1	E	53	ILE
1	E	106	LEU
1	E	134	LEU
1	E	157	ARG
1	E	225	LEU
1	E	234	ASP
1	E	319	ILE
1	E	370	ASP
1	E	421	ILE
1	E	470	ASP
1	E	507	LEU
1	E	520	ILE
1	E	557	LEU
2	F	76	LEU
2	F	91	LEU
2	F	96	LYS
2	F	106	LEU
2	F	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	230	ASN
1	A	289	HIS
1	A	297	GLN
1	A	317	ASN
1	A	325	GLN
1	A	362	GLN
1	A	373	GLN
1	A	378	ASN
1	A	390	HIS
1	A	428	GLN
1	A	491	HIS
1	A	567	ASN
2	B	73	GLN
2	B	98	HIS
2	B	135	HIS
1	C	136	GLN
1	C	145	ASN
1	C	258	GLN
1	C	273	ASN

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Mol	Chain	Res	Type
1	C	297	GLN
1	C	317	ASN
1	C	362	GLN
1	C	373	GLN
1	C	390	HIS
1	C	501	GLN
1	C	518	ASN
1	C	567	ASN
2	D	73	GLN
1	E	7	ASN
1	E	11	HIS
1	E	73	ASN
1	E	93	ASN
1	E	133	GLN
1	E	136	GLN
1	E	273	ASN
1	E	297	GLN
1	E	317	ASN
1	E	450	GLN
1	E	491	HIS
1	E	567	ASN
2	F	135	HIS

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

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, 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	564/599 (94%)	0.26	18 (3%)	50	30	65, 110, 152, 179	0
1	C	562/599 (93%)	0.27	16 (2%)	55	34	57, 121, 165, 194	0
1	E	566/599 (94%)	0.37	22 (3%)	43	24	58, 115, 183, 209	0
2	B	84/111 (75%)	0.44	2 (2%)	59	38	132, 174, 196, 201	0
2	D	82/111 (73%)	0.39	3 (3%)	45	25	154, 169, 191, 203	0
2	F	71/111 (63%)	0.70	5 (7%)	22	12	151, 160, 172, 188	0
All	All	1929/2130 (90%)	0.32	66 (3%)	48	28	57, 119, 181, 209	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	ASP	4.3
1	E	507	LEU	4.2
1	C	-2	GLN	4.1
1	E	511	ASP	4.0
2	D	75	LEU	3.9
1	A	319	ILE	3.7
1	C	260	LEU	3.6
1	A	416	HIS	3.5
1	A	510	LEU	3.5
1	E	-5	VAL	3.3
1	C	507	LEU	3.2
1	E	-7	LEU	3.2
1	E	510	LEU	3.2
1	A	557	LEU	3.1
2	F	130	VAL	3.0
2	F	138	THR	2.9
1	E	101	LEU	2.9
1	E	5	GLU	2.9
1	E	75	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	-10	SER	2.8
2	B	103	THR	2.8
1	E	547	CYS	2.8
1	C	472	PHE	2.8
1	A	357	ILE	2.8
1	E	512	ILE	2.7
1	E	558	PHE	2.6
1	C	323	LEU	2.6
1	E	497	VAL	2.6
2	F	139	VAL	2.6
2	F	84	LEU	2.5
1	A	309	GLU	2.5
1	C	562	LEU	2.5
1	C	463	PHE	2.5
1	C	466	GLN	2.5
1	A	504	SER	2.4
2	D	130	VAL	2.3
1	C	29	SER	2.3
1	C	513	ILE	2.3
1	E	419	LEU	2.3
1	A	-2	GLN	2.3
1	A	501	GLN	2.2
1	E	414	LEU	2.2
1	E	501	GLN	2.2
1	E	543	ILE	2.2
2	D	114	LEU	2.2
1	C	561	ILE	2.1
1	C	419	LEU	2.1
2	B	75	LEU	2.1
1	A	242	VAL	2.1
1	E	393	VAL	2.1
1	A	421	ILE	2.1
1	E	516	PHE	2.1
1	A	-13	HIS	2.1
1	A	74	ILE	2.1
1	E	494	PHE	2.1
2	F	94	LYS	2.1
1	A	151	ILE	2.1
1	A	254	ASP	2.1
1	A	547	CYS	2.1
1	C	508	PHE	2.1
1	C	540	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	421	ILE	2.0
1	C	516	PHE	2.0
1	E	104	PHE	2.0
1	E	557	LEU	2.0
1	C	167	ILE	2.0

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.