wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:41 PM GMT

PDB ID	:	4V81
Title	:	The crystal structure of yeast CCT reveals intrinsic asymmetry of eukaryotic cytosolic chaperonins
Authors	:	Dekker, C.; Roe, S.M.; McCormack, E.A.; Beuron, F.; Pearl, L.H.; Willison, K.R.
Deposited on	:	2010-10-17
Resolution	:	3.80 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
http://wwpdb.org/validation/2016/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:

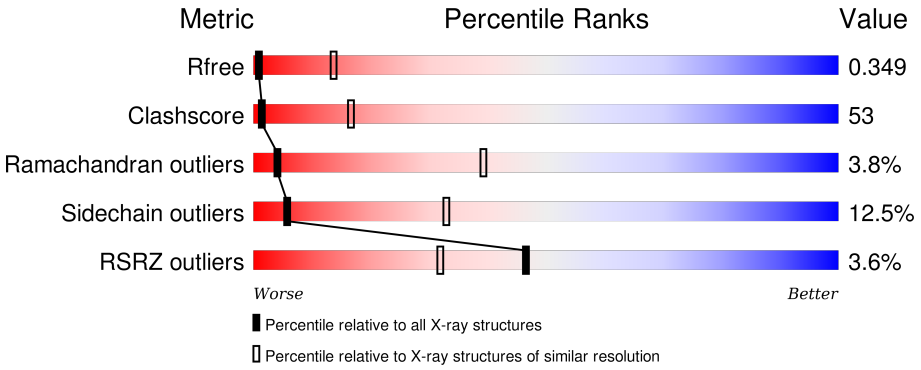
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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. 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	559	2% 52% 39% 6%
1	I	559	5% 53% 38% 6%
1	a	559	3% 89% 8%
1	i	559	3% 89% 8%
2	B	527	% 36% 49% 11%

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Mol	Chain	Length	Quality of chain
2	J	527	4% 34% 51% 12%
2	b	527	2% 82% 14%
2	j	527	% 82% 14%
3	C	590	2% 45% 37% 5% 13%
3	K	590	3% 46% 36% 5% 13%
3	c	590	3% 79% 7% 13%
3	k	590	2% 79% 8% 13%
4	D	528	3% 50% 43% 6%
4	L	528	5% 50% 43% 5%
4	d	528	3% 91% 8%
4	l	528	4% 91% 8%
5	E	562	3% 48% 39% 6% 7%
5	M	562	6% 48% 39% 6% 7%
5	e	562	4% 84% 9% 7%
5	m	562	3% 84% 9% 7%
6	F	546	5% 35% 50% 12%
6	N	546	3% 37% 49% 11%
6	f	546	4% 83% 14%
6	n	546	4% 84% 14%
7	G	550	2% 43% 41% 8% 7%
7	O	550	4% 45% 40% 8% 7%
7	g	550	3% 83% 10% 7%
7	o	550	4% 83% 10% 7%
8	H	568	2% 46% 39% 7% 8%
8	P	568	7% 47% 38% 7% 8%

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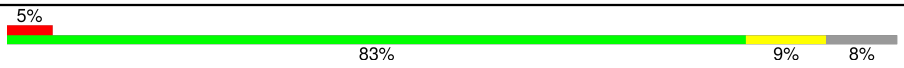
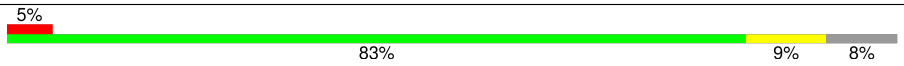
Mol	Chain	Length	Quality of chain
8	h	568	
8	p	568	

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
10	BEF	B	602	-	-	-	X
10	BEF	C	1102	-	-	X	-
10	BEF	E	602	-	-	-	X
10	BEF	F	602	-	-	X	-
10	BEF	G	602	-	-	-	X
10	BEF	N	602	-	-	X	-
9	ADP	A	601	X	-	-	-
9	ADP	B	601	X	-	-	-
9	ADP	C	1101	X	-	-	-
9	ADP	D	601	X	-	-	-
9	ADP	E	601	X	-	-	-
9	ADP	G	601	X	-	-	-
9	ADP	H	601	X	-	-	-
9	ADP	J	601	X	-	-	-
9	ADP	M	601	X	-	-	-
9	ADP	N	601	X	-	-	-
9	ADP	P	601	X	-	-	-
9	ADP	a	1601	X	-	-	-
9	ADP	b	1601	X	-	-	-
9	ADP	e	1601	X	-	-	-
9	ADP	f	1601	X	-	-	-
9	ADP	g	1601	X	-	-	-
9	ADP	h	1601	X	-	-	-
9	ADP	k	2101	X	-	-	-
9	ADP	m	1601	X	-	-	-
9	ADP	n	1601	X	-	-	-
9	ADP	p	1601	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 111235 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	I	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	a	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	i	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	513	Total	C	N	O	S	0	0	0
			3459	2125	597	728	9			
2	J	513	Total	C	N	O	S	0	0	0
			3459	2125	597	728	9			
2	b	513	Total	C	N	O	S	0	0	0
			3460	2126	597	728	9			
2	j	513	Total	C	N	O	S	0	0	0
			3457	2123	597	728	9			

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	514	Total	C	N	O	S	0	0	0
			3392	2104	590	685	13			
3	K	514	Total	C	N	O	S	0	0	0
			3393	2104	590	685	14			
3	c	514	Total	C	N	O	S	0	0	0
			3395	2106	590	685	14			
3	k	514	Total	C	N	O	S	0	0	0
			3395	2106	590	685	14			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1001	GLY	-	SEE REMARK 999	UNP P39077
C	1002	SER	-	SEE REMARK 999	UNP P39077
C	1003	GLY	-	SEE REMARK 999	UNP P39077
C	1004	SER	-	SEE REMARK 999	UNP P39077
C	1005	GLY	-	SEE REMARK 999	UNP P39077
C	1006	TRP	-	SEE REMARK 999	UNP P39077
C	1007	SER	-	SEE REMARK 999	UNP P39077
C	1008	HIS	-	SEE REMARK 999	UNP P39077
C	1009	PRO	-	SEE REMARK 999	UNP P39077
C	1010	GLN	-	SEE REMARK 999	UNP P39077
C	1011	PHE	-	SEE REMARK 999	UNP P39077
C	1012	GLU	-	SEE REMARK 999	UNP P39077
C	1013	LYS	-	SEE REMARK 999	UNP P39077
C	1014	GLY	-	SEE REMARK 999	UNP P39077
C	1015	SER	-	SEE REMARK 999	UNP P39077
C	1016	GLY	-	SEE REMARK 999	UNP P39077
C	1017	LYS	-	SEE REMARK 999	UNP P39077
C	1018	ARG	-	SEE REMARK 999	UNP P39077
C	1019	ARG	-	SEE REMARK 999	UNP P39077
C	1020	TRP	-	SEE REMARK 999	UNP P39077
C	1021	LYS	-	SEE REMARK 999	UNP P39077
C	1022	LYS	-	SEE REMARK 999	UNP P39077
C	1023	ASN	-	SEE REMARK 999	UNP P39077
C	1024	PHE	-	SEE REMARK 999	UNP P39077
C	1025	ILE	-	SEE REMARK 999	UNP P39077
C	1026	ALA	-	SEE REMARK 999	UNP P39077
C	1027	VAL	-	SEE REMARK 999	UNP P39077
C	1028	SER	-	SEE REMARK 999	UNP P39077
C	1029	ALA	-	SEE REMARK 999	UNP P39077
C	1030	ALA	-	SEE REMARK 999	UNP P39077
C	1031	ASN	-	SEE REMARK 999	UNP P39077
C	1032	ARG	-	SEE REMARK 999	UNP P39077
C	1033	PHE	-	SEE REMARK 999	UNP P39077
C	1034	LYS	-	SEE REMARK 999	UNP P39077
C	1035	LYS	-	SEE REMARK 999	UNP P39077
C	1036	ILE	-	SEE REMARK 999	UNP P39077
C	1037	SER	-	SEE REMARK 999	UNP P39077
C	1038	SER	-	SEE REMARK 999	UNP P39077
C	1039	SER	-	SEE REMARK 999	UNP P39077
C	1040	GLY	-	SEE REMARK 999	UNP P39077
C	1041	ALA	-	SEE REMARK 999	UNP P39077
C	1042	LEU	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1043	GLY	-	SEE REMARK 999	UNP P39077
C	1044	SER	-	SEE REMARK 999	UNP P39077
C	1045	GLY	-	SEE REMARK 999	UNP P39077
C	1046	HIS	-	SEE REMARK 999	UNP P39077
C	1047	HIS	-	SEE REMARK 999	UNP P39077
C	1048	HIS	-	SEE REMARK 999	UNP P39077
C	1049	HIS	-	SEE REMARK 999	UNP P39077
C	1050	HIS	-	SEE REMARK 999	UNP P39077
C	1051	HIS	-	SEE REMARK 999	UNP P39077
C	1052	HIS	-	SEE REMARK 999	UNP P39077
C	1053	HIS	-	SEE REMARK 999	UNP P39077
C	1054	GLY	-	SEE REMARK 999	UNP P39077
C	1055	SER	-	SEE REMARK 999	UNP P39077
C	1056	GLY	-	SEE REMARK 999	UNP P39077
K	1001	GLY	-	SEE REMARK 999	UNP P39077
K	1002	SER	-	SEE REMARK 999	UNP P39077
K	1003	GLY	-	SEE REMARK 999	UNP P39077
K	1004	SER	-	SEE REMARK 999	UNP P39077
K	1005	GLY	-	SEE REMARK 999	UNP P39077
K	1006	TRP	-	SEE REMARK 999	UNP P39077
K	1007	SER	-	SEE REMARK 999	UNP P39077
K	1008	HIS	-	SEE REMARK 999	UNP P39077
K	1009	PRO	-	SEE REMARK 999	UNP P39077
K	1010	GLN	-	SEE REMARK 999	UNP P39077
K	1011	PHE	-	SEE REMARK 999	UNP P39077
K	1012	GLU	-	SEE REMARK 999	UNP P39077
K	1013	LYS	-	SEE REMARK 999	UNP P39077
K	1014	GLY	-	SEE REMARK 999	UNP P39077
K	1015	SER	-	SEE REMARK 999	UNP P39077
K	1016	GLY	-	SEE REMARK 999	UNP P39077
K	1017	LYS	-	SEE REMARK 999	UNP P39077
K	1018	ARG	-	SEE REMARK 999	UNP P39077
K	1019	ARG	-	SEE REMARK 999	UNP P39077
K	1020	TRP	-	SEE REMARK 999	UNP P39077
K	1021	LYS	-	SEE REMARK 999	UNP P39077
K	1022	LYS	-	SEE REMARK 999	UNP P39077
K	1023	ASN	-	SEE REMARK 999	UNP P39077
K	1024	PHE	-	SEE REMARK 999	UNP P39077
K	1025	ILE	-	SEE REMARK 999	UNP P39077
K	1026	ALA	-	SEE REMARK 999	UNP P39077
K	1027	VAL	-	SEE REMARK 999	UNP P39077
K	1028	SER	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1029	ALA	-	SEE REMARK 999	UNP P39077
K	1030	ALA	-	SEE REMARK 999	UNP P39077
K	1031	ASN	-	SEE REMARK 999	UNP P39077
K	1032	ARG	-	SEE REMARK 999	UNP P39077
K	1033	PHE	-	SEE REMARK 999	UNP P39077
K	1034	LYS	-	SEE REMARK 999	UNP P39077
K	1035	LYS	-	SEE REMARK 999	UNP P39077
K	1036	ILE	-	SEE REMARK 999	UNP P39077
K	1037	SER	-	SEE REMARK 999	UNP P39077
K	1038	SER	-	SEE REMARK 999	UNP P39077
K	1039	SER	-	SEE REMARK 999	UNP P39077
K	1040	GLY	-	SEE REMARK 999	UNP P39077
K	1041	ALA	-	SEE REMARK 999	UNP P39077
K	1042	LEU	-	SEE REMARK 999	UNP P39077
K	1043	GLY	-	SEE REMARK 999	UNP P39077
K	1044	SER	-	SEE REMARK 999	UNP P39077
K	1045	GLY	-	SEE REMARK 999	UNP P39077
K	1046	HIS	-	SEE REMARK 999	UNP P39077
K	1047	HIS	-	SEE REMARK 999	UNP P39077
K	1048	HIS	-	SEE REMARK 999	UNP P39077
K	1049	HIS	-	SEE REMARK 999	UNP P39077
K	1050	HIS	-	SEE REMARK 999	UNP P39077
K	1051	HIS	-	SEE REMARK 999	UNP P39077
K	1052	HIS	-	SEE REMARK 999	UNP P39077
K	1053	HIS	-	SEE REMARK 999	UNP P39077
K	1054	GLY	-	SEE REMARK 999	UNP P39077
K	1055	SER	-	SEE REMARK 999	UNP P39077
K	1056	GLY	-	SEE REMARK 999	UNP P39077
c	2001	GLY	-	SEE REMARK 999	UNP P39077
c	2002	SER	-	SEE REMARK 999	UNP P39077
c	2003	GLY	-	SEE REMARK 999	UNP P39077
c	2004	SER	-	SEE REMARK 999	UNP P39077
c	2005	GLY	-	SEE REMARK 999	UNP P39077
c	2006	TRP	-	SEE REMARK 999	UNP P39077
c	2007	SER	-	SEE REMARK 999	UNP P39077
c	2008	HIS	-	SEE REMARK 999	UNP P39077
c	2009	PRO	-	SEE REMARK 999	UNP P39077
c	2010	GLN	-	SEE REMARK 999	UNP P39077
c	2011	PHE	-	SEE REMARK 999	UNP P39077
c	2012	GLU	-	SEE REMARK 999	UNP P39077
c	2013	LYS	-	SEE REMARK 999	UNP P39077
c	2014	GLY	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
c	2015	SER	-	SEE REMARK 999	UNP P39077
c	2016	GLY	-	SEE REMARK 999	UNP P39077
c	2017	LYS	-	SEE REMARK 999	UNP P39077
c	2018	ARG	-	SEE REMARK 999	UNP P39077
c	2019	ARG	-	SEE REMARK 999	UNP P39077
c	2020	TRP	-	SEE REMARK 999	UNP P39077
c	2021	LYS	-	SEE REMARK 999	UNP P39077
c	2022	LYS	-	SEE REMARK 999	UNP P39077
c	2023	ASN	-	SEE REMARK 999	UNP P39077
c	2024	PHE	-	SEE REMARK 999	UNP P39077
c	2025	ILE	-	SEE REMARK 999	UNP P39077
c	2026	ALA	-	SEE REMARK 999	UNP P39077
c	2027	VAL	-	SEE REMARK 999	UNP P39077
c	2028	SER	-	SEE REMARK 999	UNP P39077
c	2029	ALA	-	SEE REMARK 999	UNP P39077
c	2030	ALA	-	SEE REMARK 999	UNP P39077
c	2031	ASN	-	SEE REMARK 999	UNP P39077
c	2032	ARG	-	SEE REMARK 999	UNP P39077
c	2033	PHE	-	SEE REMARK 999	UNP P39077
c	2034	LYS	-	SEE REMARK 999	UNP P39077
c	2035	LYS	-	SEE REMARK 999	UNP P39077
c	2036	ILE	-	SEE REMARK 999	UNP P39077
c	2037	SER	-	SEE REMARK 999	UNP P39077
c	2038	SER	-	SEE REMARK 999	UNP P39077
c	2039	SER	-	SEE REMARK 999	UNP P39077
c	2040	GLY	-	SEE REMARK 999	UNP P39077
c	2041	ALA	-	SEE REMARK 999	UNP P39077
c	2042	LEU	-	SEE REMARK 999	UNP P39077
c	2043	GLY	-	SEE REMARK 999	UNP P39077
c	2044	SER	-	SEE REMARK 999	UNP P39077
c	2045	GLY	-	SEE REMARK 999	UNP P39077
c	2046	HIS	-	SEE REMARK 999	UNP P39077
c	2047	HIS	-	SEE REMARK 999	UNP P39077
c	2048	HIS	-	SEE REMARK 999	UNP P39077
c	2049	HIS	-	SEE REMARK 999	UNP P39077
c	2050	HIS	-	SEE REMARK 999	UNP P39077
c	2051	HIS	-	SEE REMARK 999	UNP P39077
c	2052	HIS	-	SEE REMARK 999	UNP P39077
c	2053	HIS	-	SEE REMARK 999	UNP P39077
c	2054	GLY	-	SEE REMARK 999	UNP P39077
c	2055	SER	-	SEE REMARK 999	UNP P39077
c	2056	GLY	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	2001	GLY	-	SEE REMARK 999	UNP P39077
k	2002	SER	-	SEE REMARK 999	UNP P39077
k	2003	GLY	-	SEE REMARK 999	UNP P39077
k	2004	SER	-	SEE REMARK 999	UNP P39077
k	2005	GLY	-	SEE REMARK 999	UNP P39077
k	2006	TRP	-	SEE REMARK 999	UNP P39077
k	2007	SER	-	SEE REMARK 999	UNP P39077
k	2008	HIS	-	SEE REMARK 999	UNP P39077
k	2009	PRO	-	SEE REMARK 999	UNP P39077
k	2010	GLN	-	SEE REMARK 999	UNP P39077
k	2011	PHE	-	SEE REMARK 999	UNP P39077
k	2012	GLU	-	SEE REMARK 999	UNP P39077
k	2013	LYS	-	SEE REMARK 999	UNP P39077
k	2014	GLY	-	SEE REMARK 999	UNP P39077
k	2015	SER	-	SEE REMARK 999	UNP P39077
k	2016	GLY	-	SEE REMARK 999	UNP P39077
k	2017	LYS	-	SEE REMARK 999	UNP P39077
k	2018	ARG	-	SEE REMARK 999	UNP P39077
k	2019	ARG	-	SEE REMARK 999	UNP P39077
k	2020	TRP	-	SEE REMARK 999	UNP P39077
k	2021	LYS	-	SEE REMARK 999	UNP P39077
k	2022	LYS	-	SEE REMARK 999	UNP P39077
k	2023	ASN	-	SEE REMARK 999	UNP P39077
k	2024	PHE	-	SEE REMARK 999	UNP P39077
k	2025	ILE	-	SEE REMARK 999	UNP P39077
k	2026	ALA	-	SEE REMARK 999	UNP P39077
k	2027	VAL	-	SEE REMARK 999	UNP P39077
k	2028	SER	-	SEE REMARK 999	UNP P39077
k	2029	ALA	-	SEE REMARK 999	UNP P39077
k	2030	ALA	-	SEE REMARK 999	UNP P39077
k	2031	ASN	-	SEE REMARK 999	UNP P39077
k	2032	ARG	-	SEE REMARK 999	UNP P39077
k	2033	PHE	-	SEE REMARK 999	UNP P39077
k	2034	LYS	-	SEE REMARK 999	UNP P39077
k	2035	LYS	-	SEE REMARK 999	UNP P39077
k	2036	ILE	-	SEE REMARK 999	UNP P39077
k	2037	SER	-	SEE REMARK 999	UNP P39077
k	2038	SER	-	SEE REMARK 999	UNP P39077
k	2039	SER	-	SEE REMARK 999	UNP P39077
k	2040	GLY	-	SEE REMARK 999	UNP P39077
k	2041	ALA	-	SEE REMARK 999	UNP P39077
k	2042	LEU	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	2043	GLY	-	SEE REMARK 999	UNP P39077
k	2044	SER	-	SEE REMARK 999	UNP P39077
k	2045	GLY	-	SEE REMARK 999	UNP P39077
k	2046	HIS	-	SEE REMARK 999	UNP P39077
k	2047	HIS	-	SEE REMARK 999	UNP P39077
k	2048	HIS	-	SEE REMARK 999	UNP P39077
k	2049	HIS	-	SEE REMARK 999	UNP P39077
k	2050	HIS	-	SEE REMARK 999	UNP P39077
k	2051	HIS	-	SEE REMARK 999	UNP P39077
k	2052	HIS	-	SEE REMARK 999	UNP P39077
k	2053	HIS	-	SEE REMARK 999	UNP P39077
k	2054	GLY	-	SEE REMARK 999	UNP P39077
k	2055	SER	-	SEE REMARK 999	UNP P39077
k	2056	GLY	-	SEE REMARK 999	UNP P39077

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	L	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	d	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	l	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
L	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
d	1345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
l	1345	ASP	GLY	ENGINEERED MUTATION	UNP P39078

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			
5	M	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	e	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			
5	m	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	533	Total	C	N	O	S	0	0	0
			3631	2253	629	740	9			
6	N	533	Total	C	N	O	S	0	0	0
			3628	2250	629	740	9			
6	f	533	Total	C	N	O	S	0	0	0
			3633	2255	630	739	9			
6	n	533	Total	C	N	O	S	0	0	0
			3629	2252	629	739	9			

- Molecule 7 is a protein called T-complex protein 1 subunit eta.

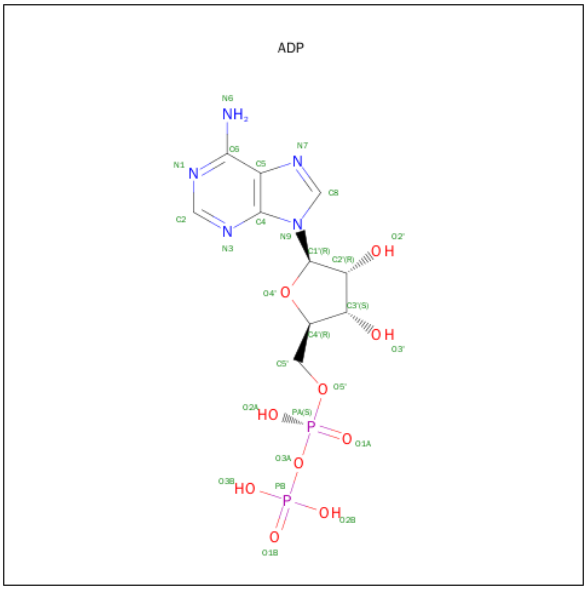
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	509	Total	C	N	O	S	0	0	0
			3317	2055	583	669	10			
7	O	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			
7	g	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			
7	o	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			
8	P	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			
8	h	525	Total	C	N	O	S	0	0	0
			3485	2159	608	705	13			
8	p	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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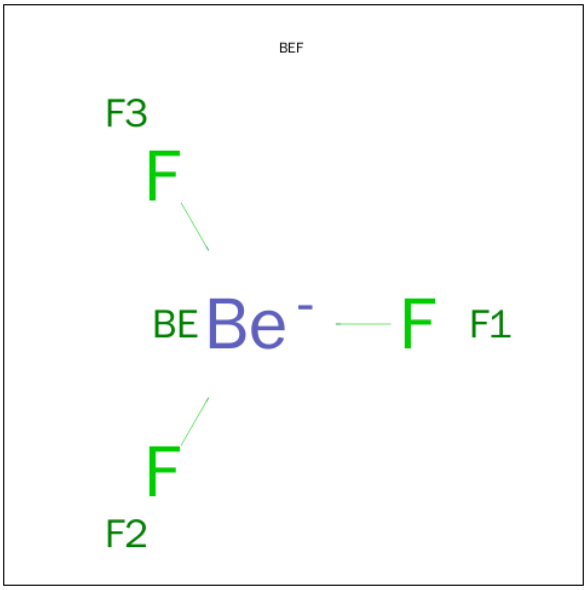
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	a	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	b	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	h	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	k	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	l	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	m	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	n	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	p	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Be F 4 1 3	0	0
10	B	1	Total Be F 4 1 3	0	0
10	C	1	Total Be F 4 1 3	0	0
10	D	1	Total Be F 4 1 3	0	0
10	E	1	Total Be F 4 1 3	0	0
10	F	1	Total Be F 4 1 3	0	0
10	G	1	Total Be F 4 1 3	0	0
10	H	1	Total Be F 4 1 3	0	0
10	J	1	Total Be F 4 1 3	0	0
10	L	1	Total Be F 4 1 3	0	0
10	M	1	Total Be F 4 1 3	0	0
10	N	1	Total Be F 4 1 3	0	0
10	P	1	Total Be F 4 1 3	0	0
10	a	1	Total Be F 4 1 3	0	0
10	b	1	Total Be F 4 1 3	0	0
10	e	1	Total Be F 4 1 3	0	0
10	f	1	Total Be F 4 1 3	0	0
10	g	1	Total Be F 4 1 3	0	0
10	h	1	Total Be F 4 1 3	0	0
10	k	1	Total Be F 4 1 3	0	0
10	l	1	Total Be F 4 1 3	0	0
10	m	1	Total Be F 4 1 3	0	0

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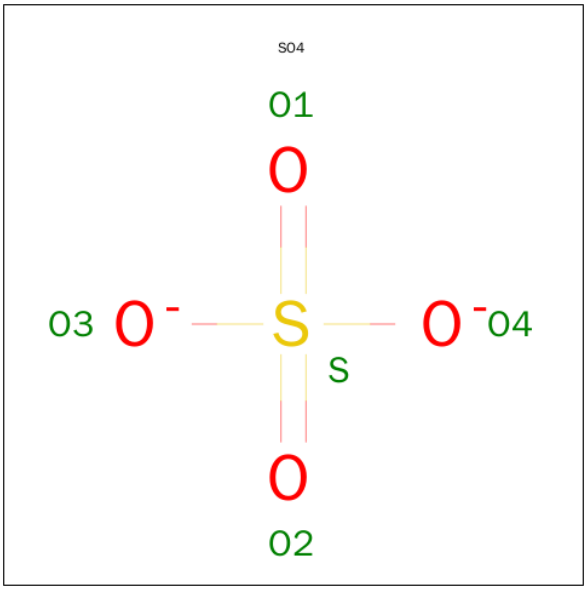
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	n	1	Total Be F 4 1 3	0	0
10	p	1	Total Be F 4 1 3	0	0

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	I	1	Total O S 5 4 1	0	0
11	K	1	Total O S 5 4 1	0	0
11	O	1	Total O S 5 4 1	0	0
11	c	1	Total O S 5 4 1	0	0
11	d	1	Total O S 5 4 1	0	0
11	i	1	Total O S 5 4 1	0	0
11	j	1	Total O S 5 4 1	0	0
11	o	1	Total O S 5 4 1	0	0

- Molecule 12 is water.

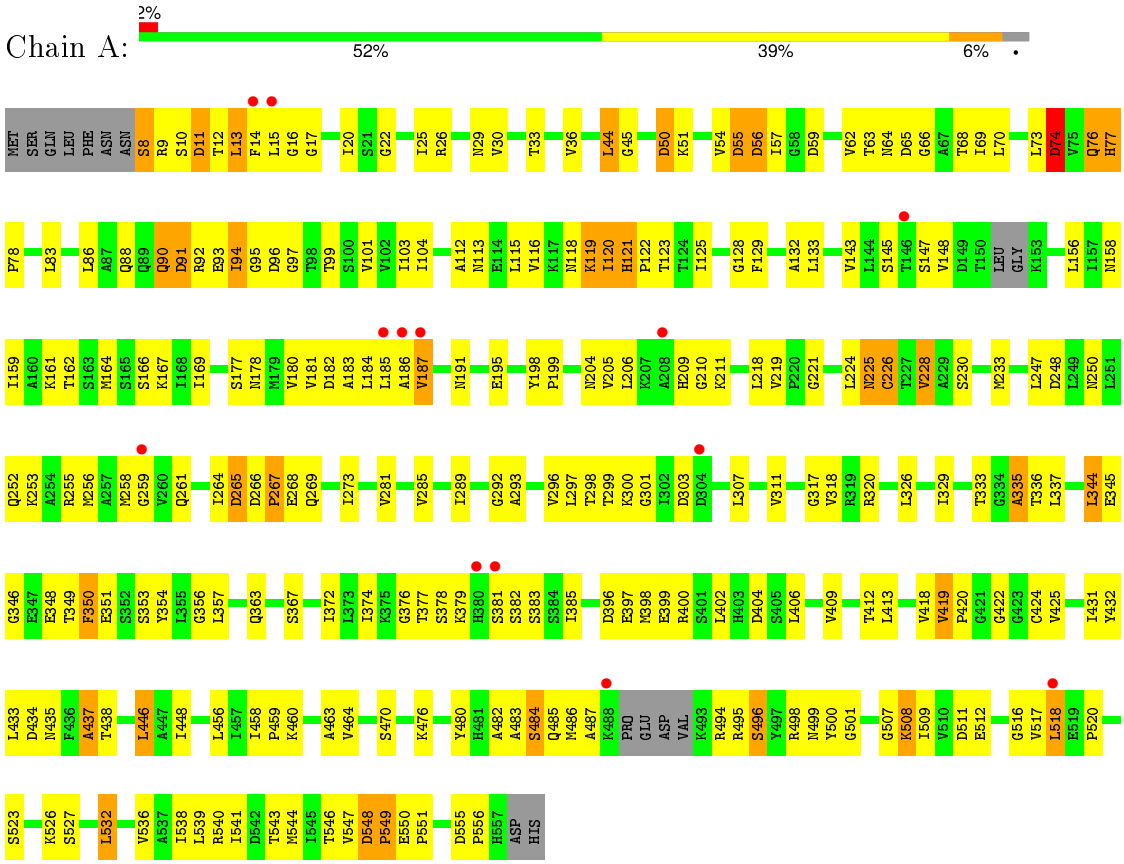
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O 1 1	0	0
12	E	1	Total O 1 1	0	0
12	G	1	Total O 1 1	0	0
12	M	1	Total O 1 1	0	0
12	e	1	Total O 1 1	0	0
12	g	1	Total O 1 1	0	0
12	m	1	Total O 1 1	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

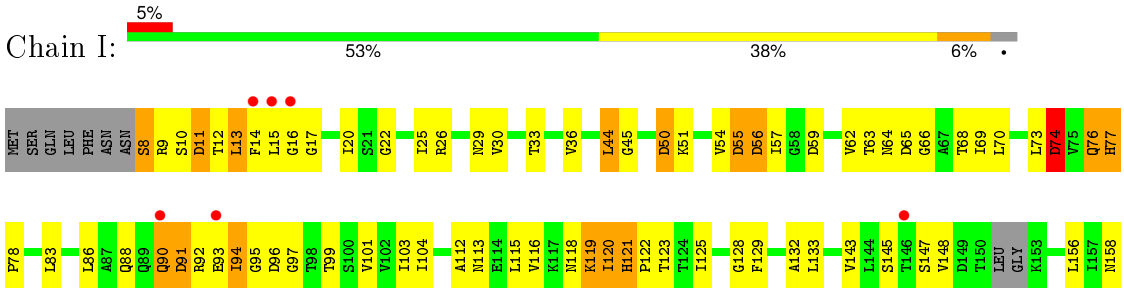
- Molecule 1: T-complex protein 1 subunit alpha

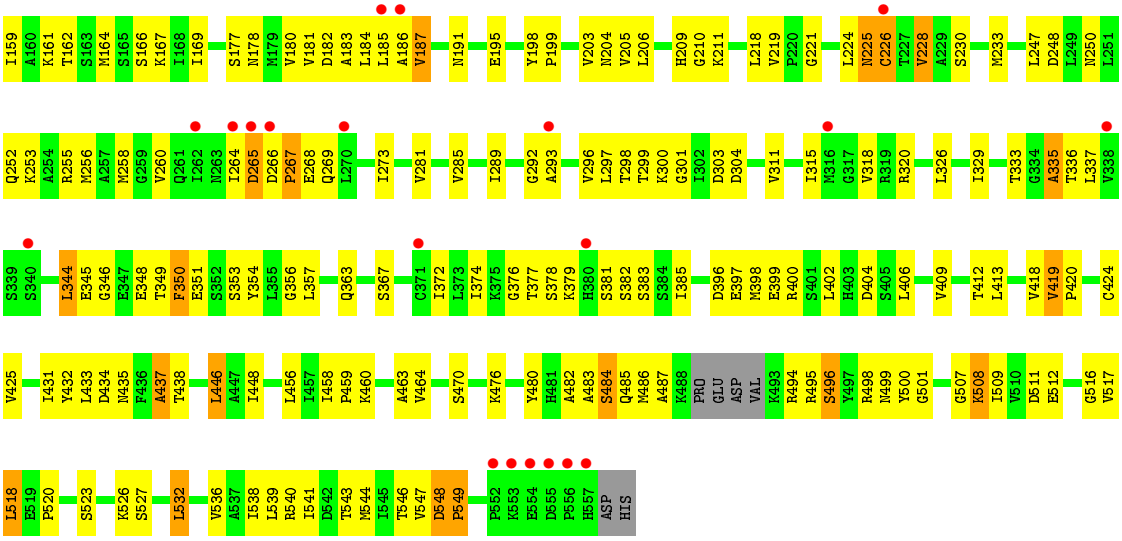
Chain A:



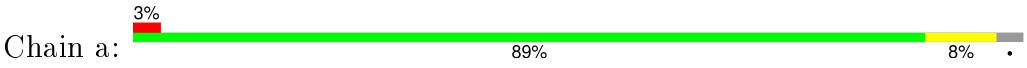
- Molecule 1: T-complex protein 1 subunit alpha

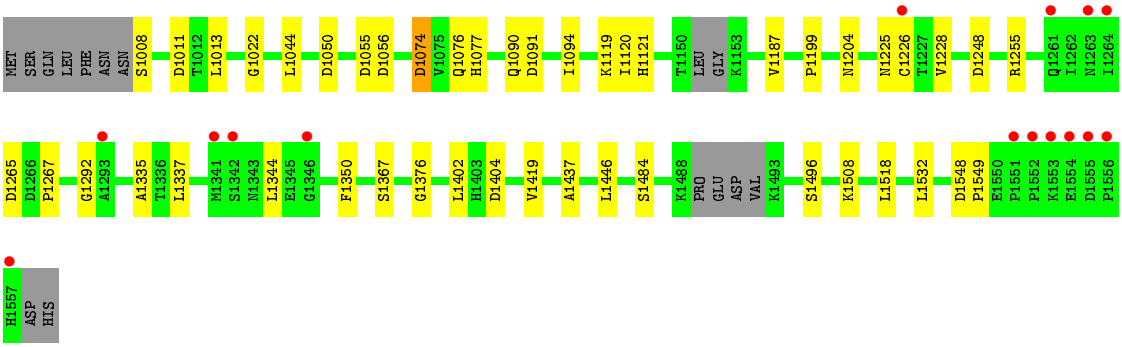
Chain I:



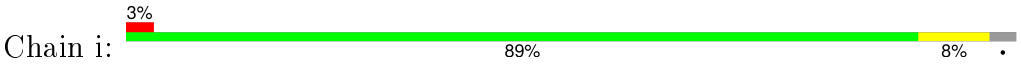


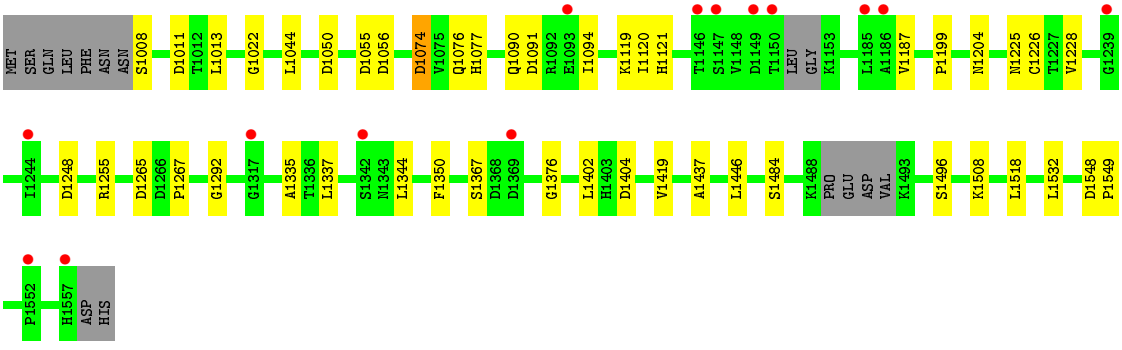
• Molecule 1: T-complex protein 1 subunit alpha



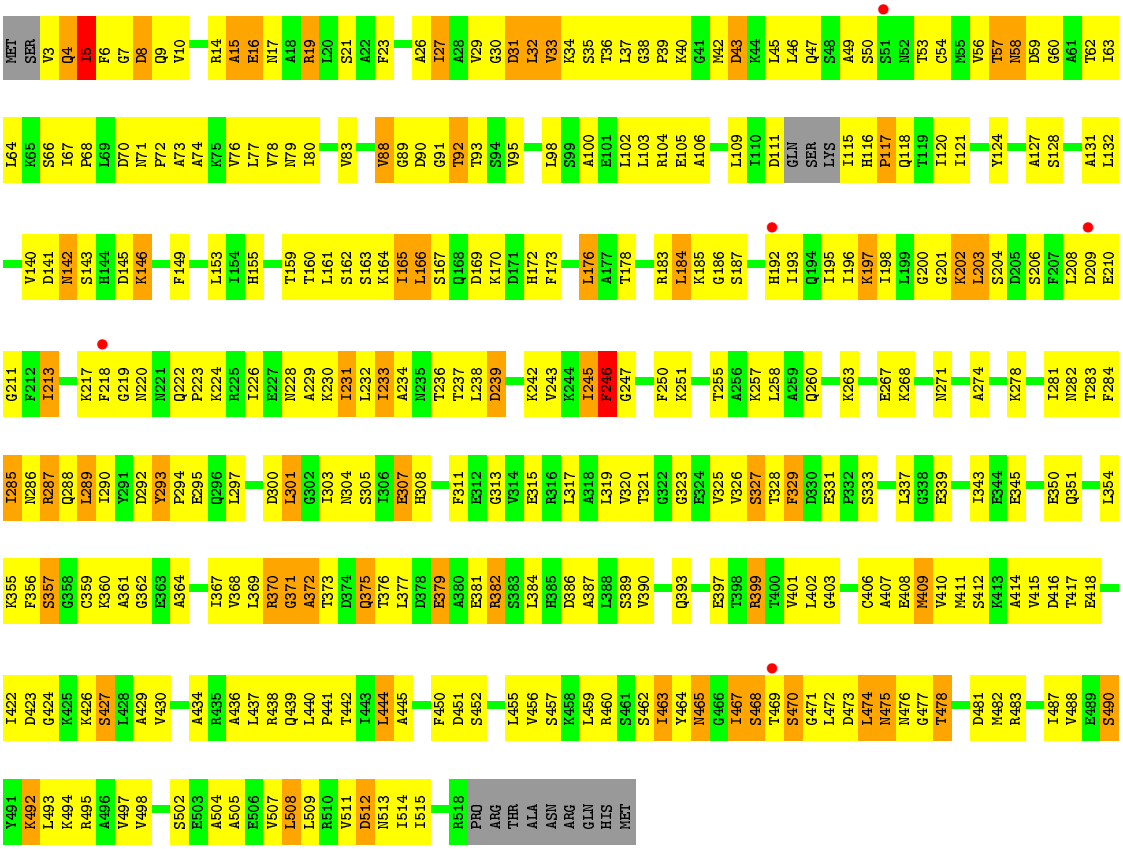


• Molecule 1: T-complex protein 1 subunit alpha



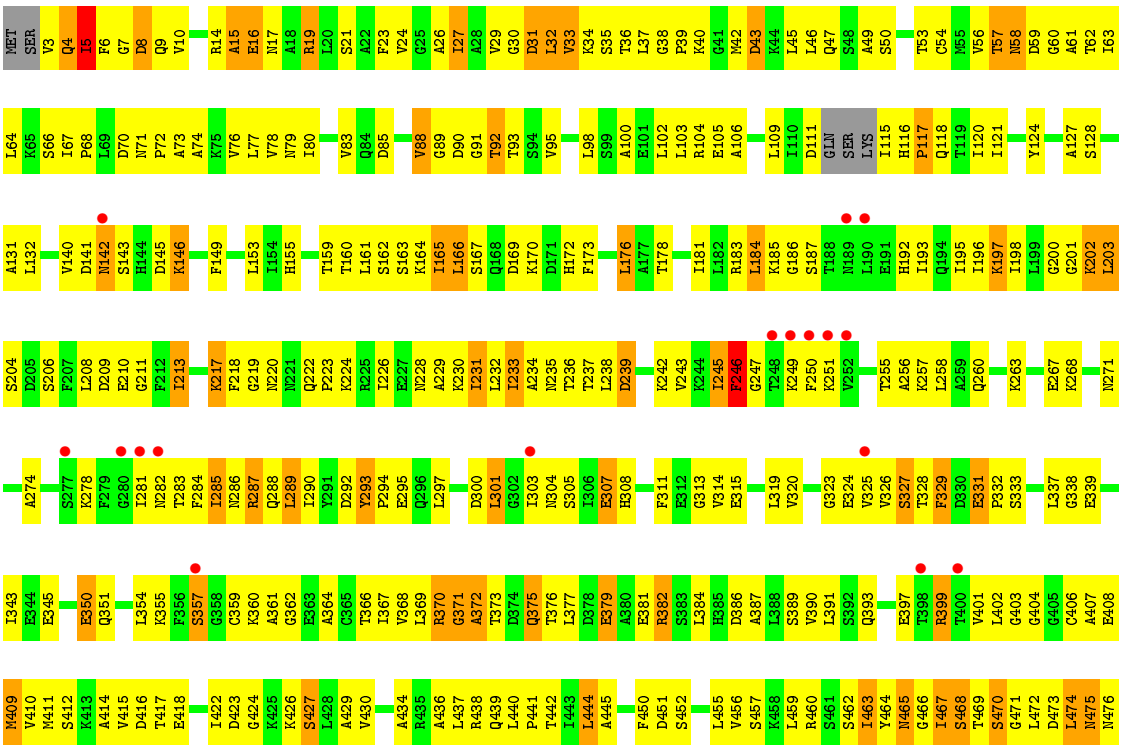


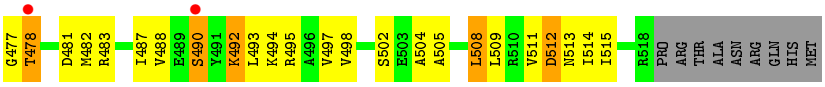
• Molecule 2: T-complex protein 1 subunit beta



- Molecule 2: T-complex protein 1 subunit beta

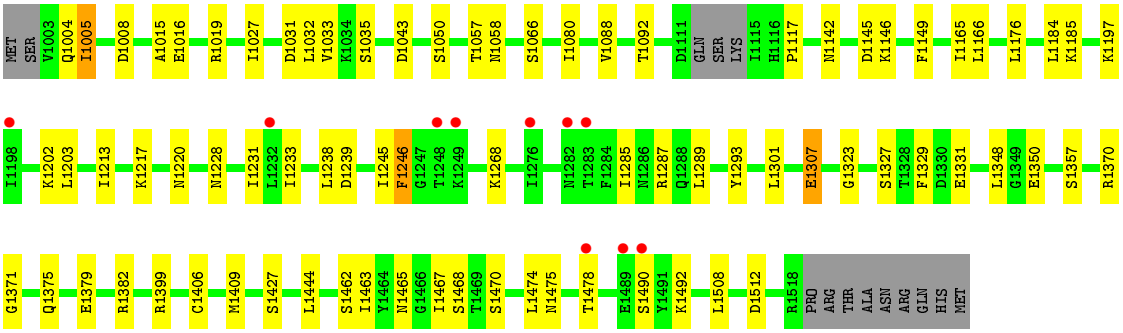
Chain J:





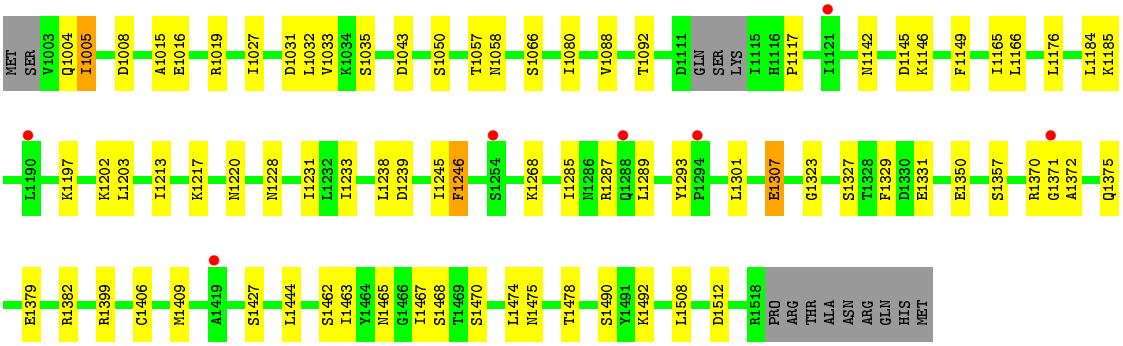
• Molecule 2: T-complex protein 1 subunit beta

Chain b:



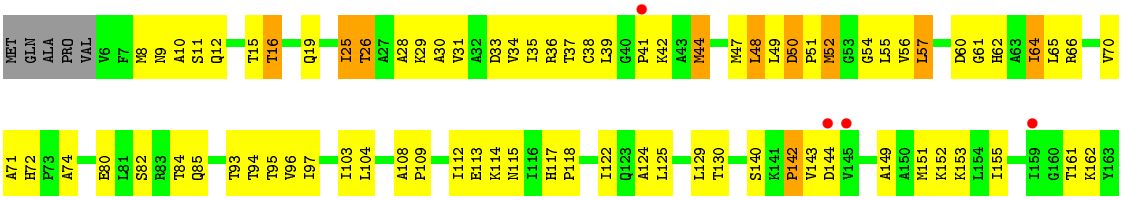
• Molecule 2: T-complex protein 1 subunit beta

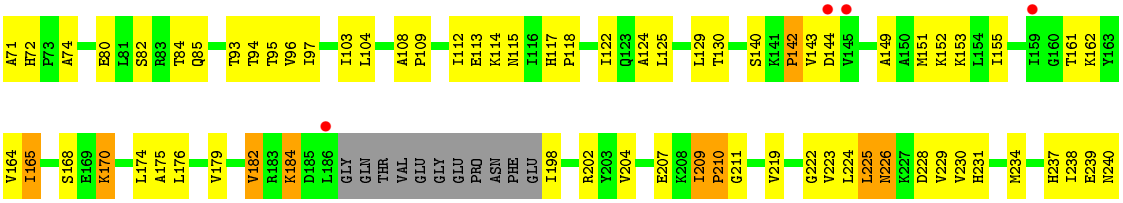
Chain j:

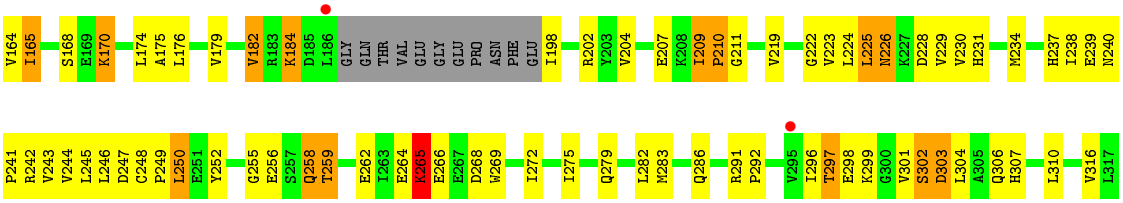


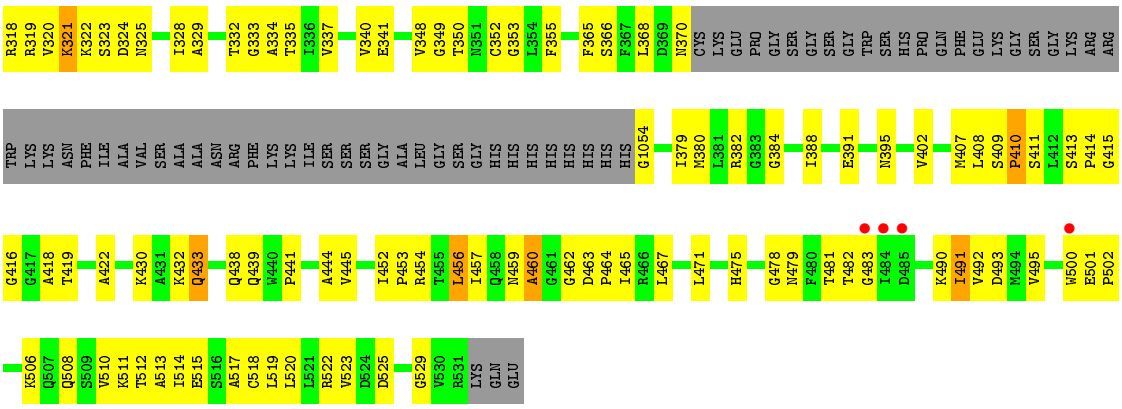
• Molecule 3: T-complex protein 1 subunit gamma

Chain C:



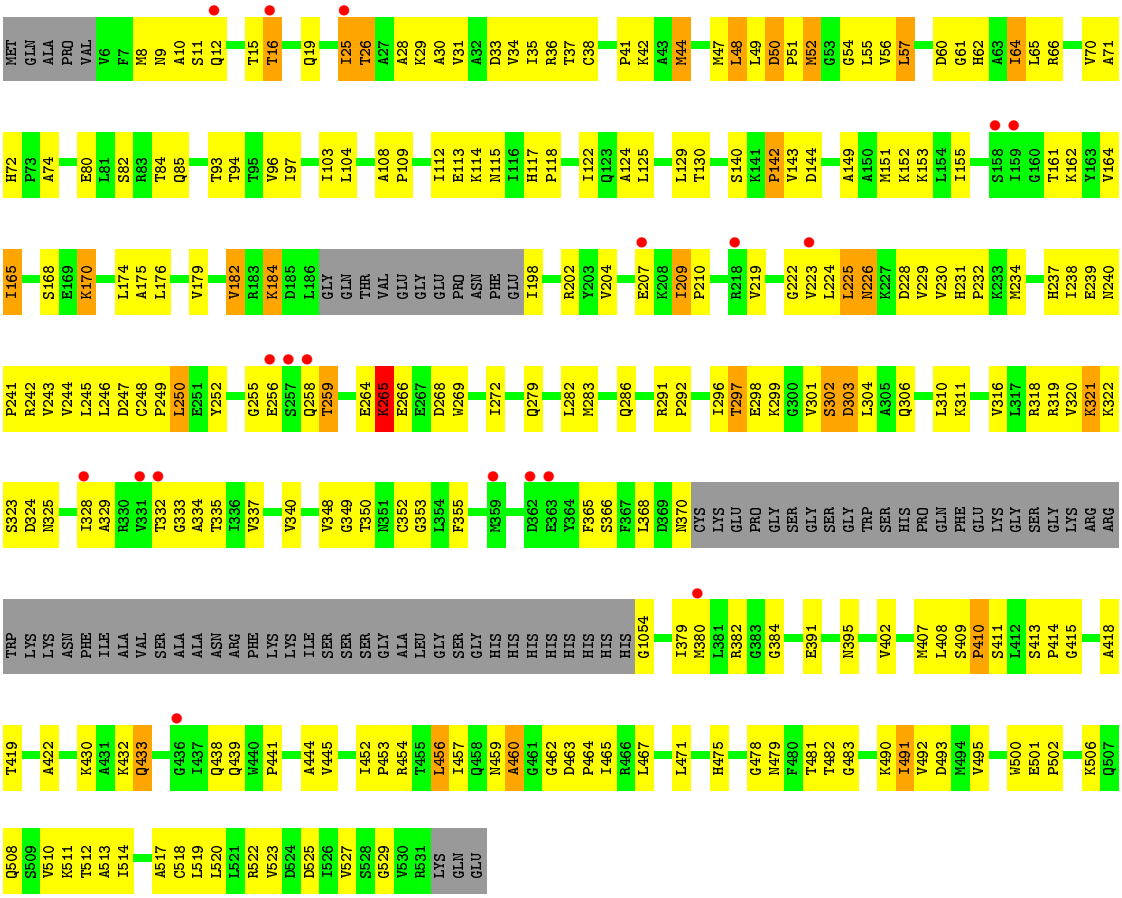






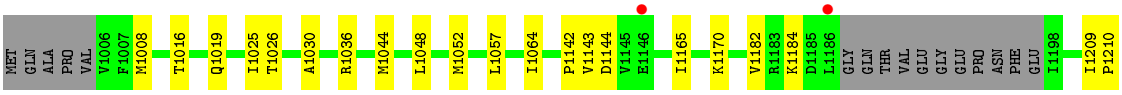
• Molecule 3: T-complex protein 1 subunit gamma

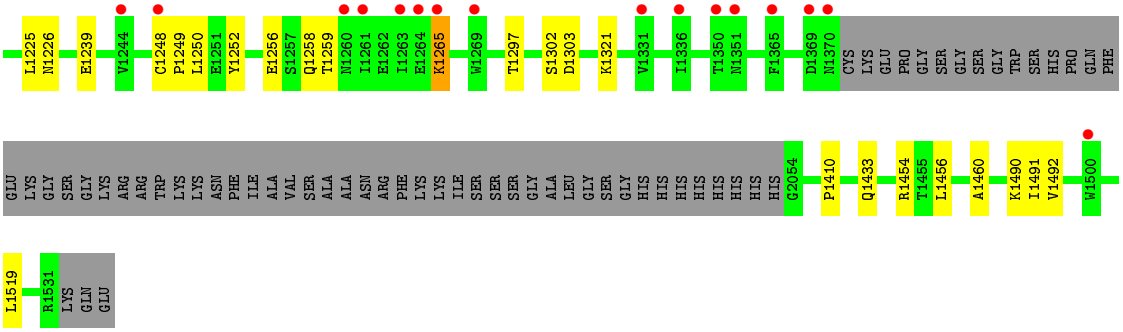
Chain K:



• Molecule 3: T-complex protein 1 subunit gamma

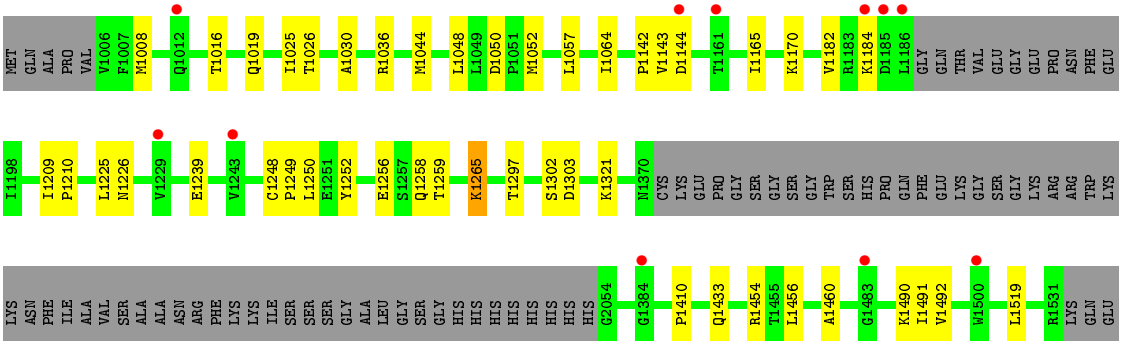
Chain c:





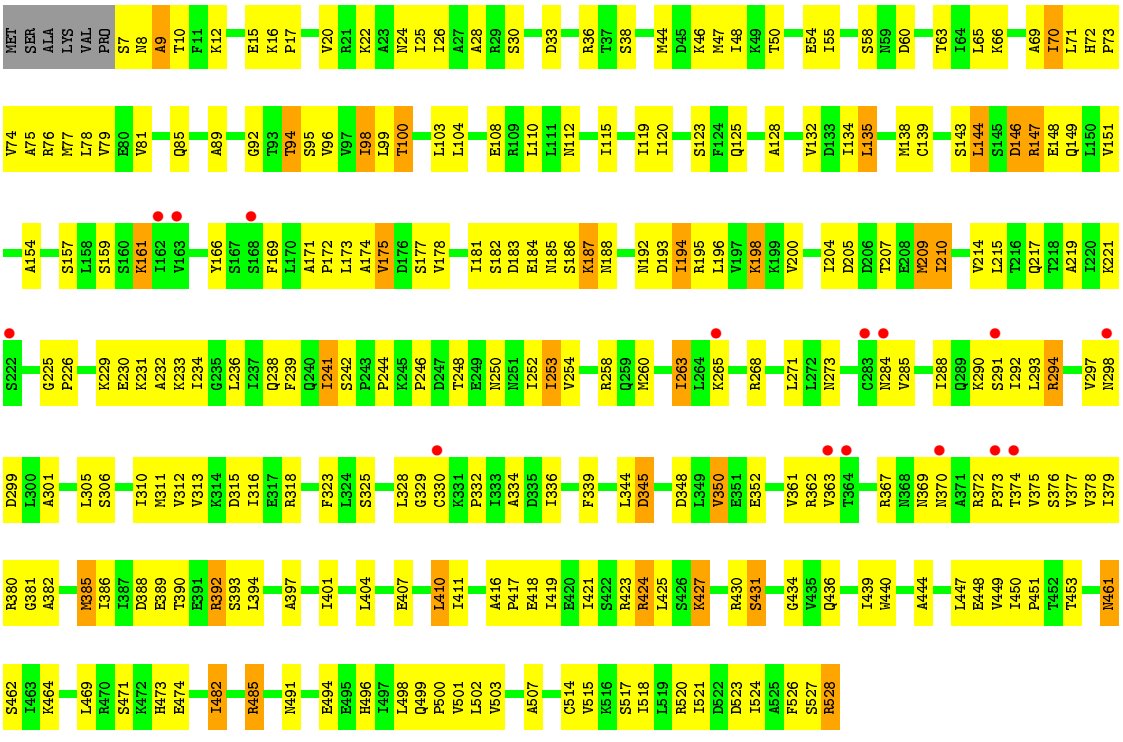
• Molecule 3: T-complex protein 1 subunit gamma

Chain k:



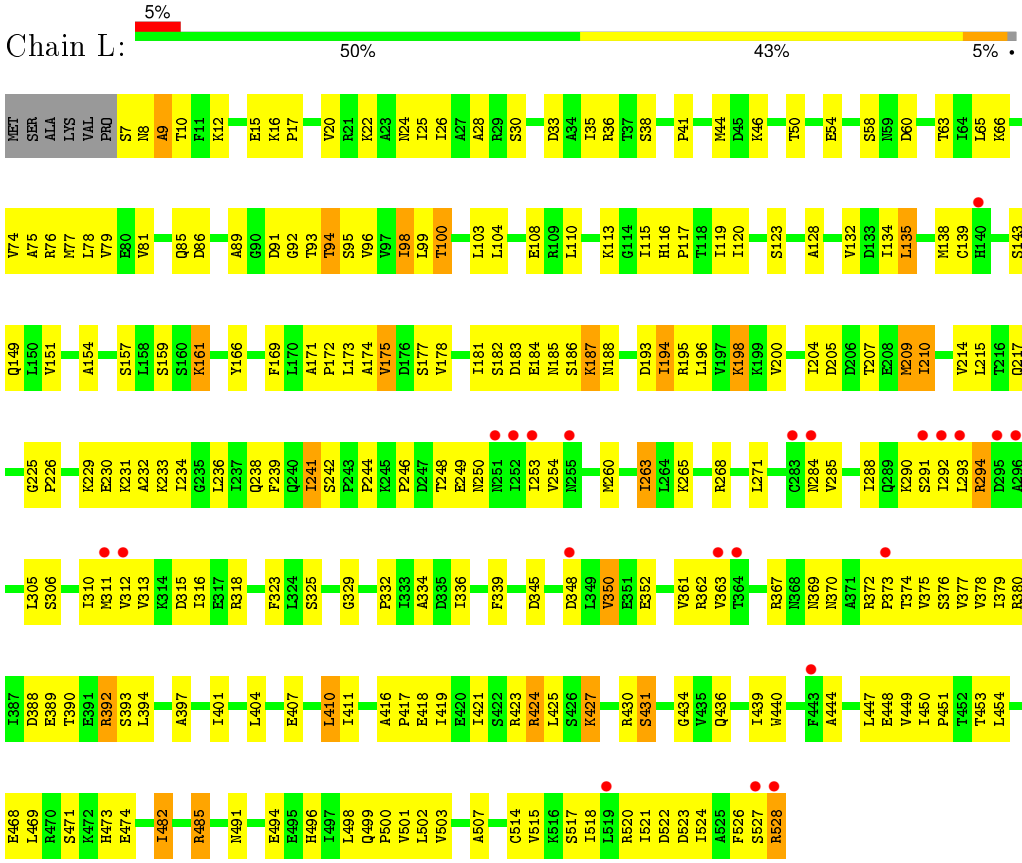
• Molecule 4: T-complex protein 1 subunit delta

Chain D:



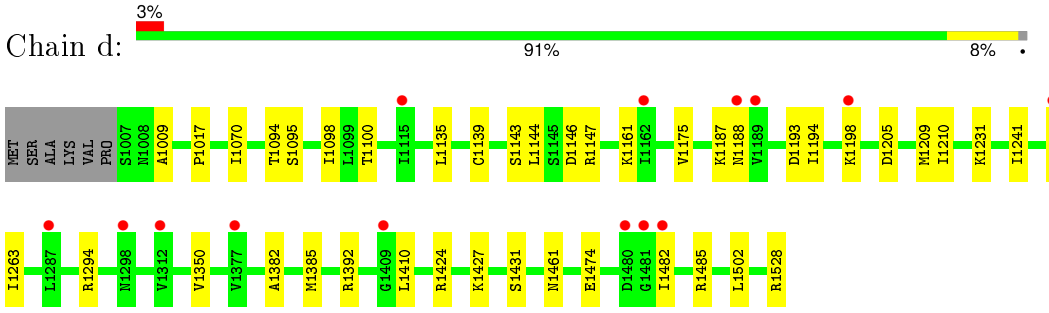
• Molecule 4: T-complex protein 1 subunit delta

Chain L:



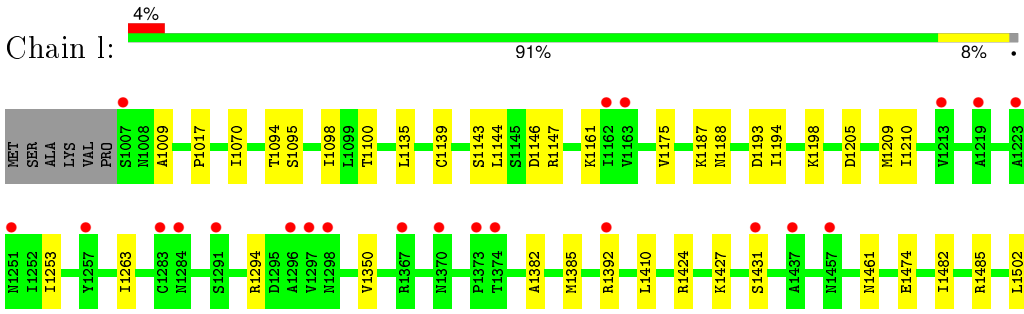
• Molecule 4: T-complex protein 1 subunit delta

Chain d:



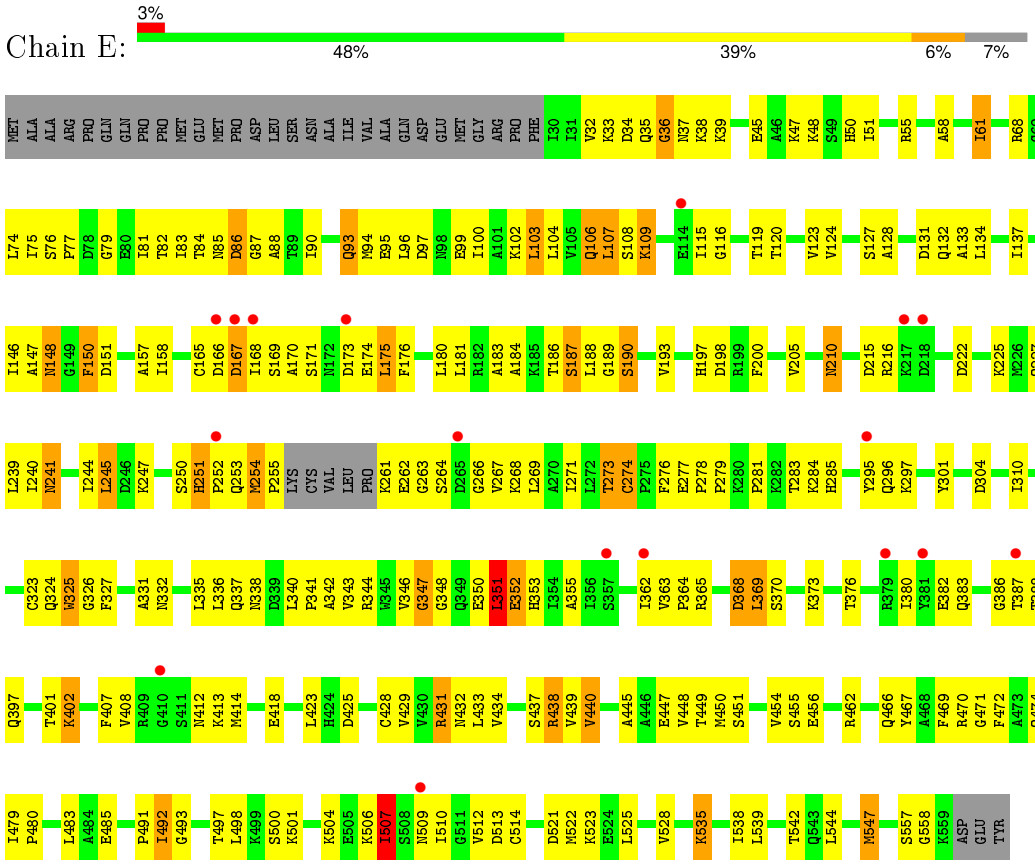
• Molecule 4: T-complex protein 1 subunit delta

Chain l:



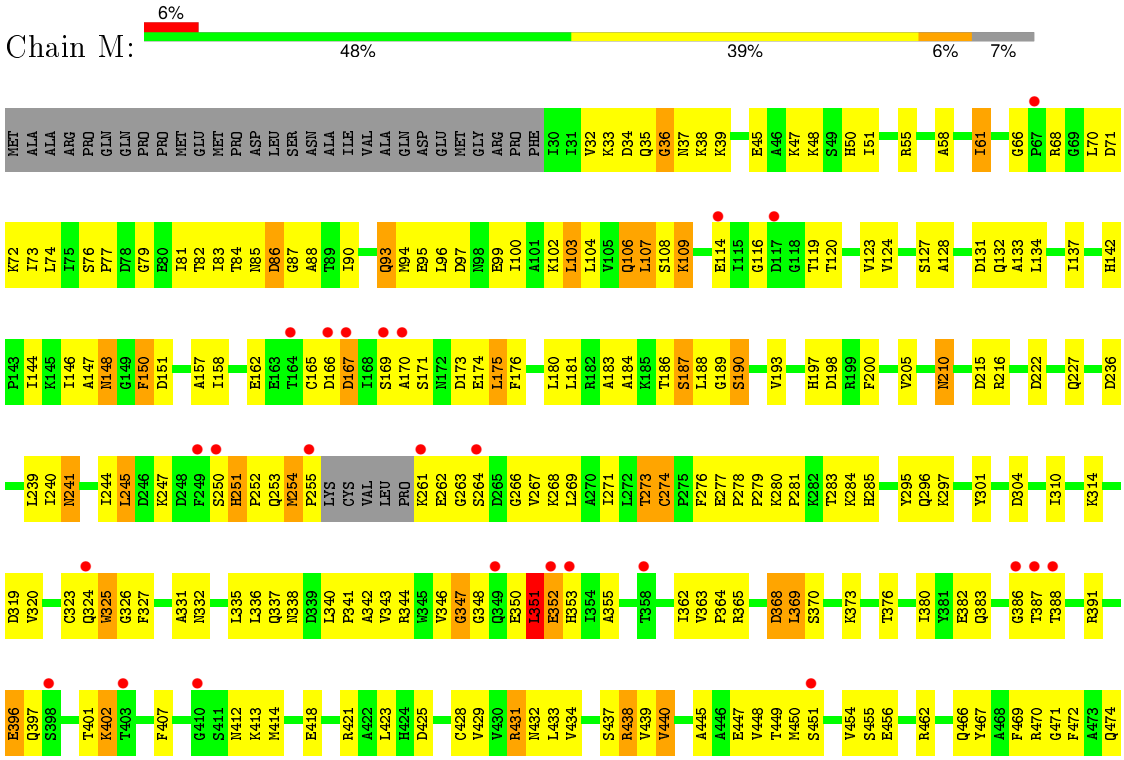
• Molecule 5: T-complex protein 1 subunit epsilon

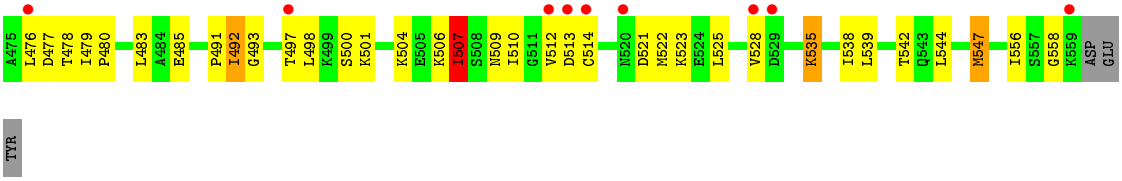
Chain E:



- Molecule 5: T-complex protein 1 subunit epsilon

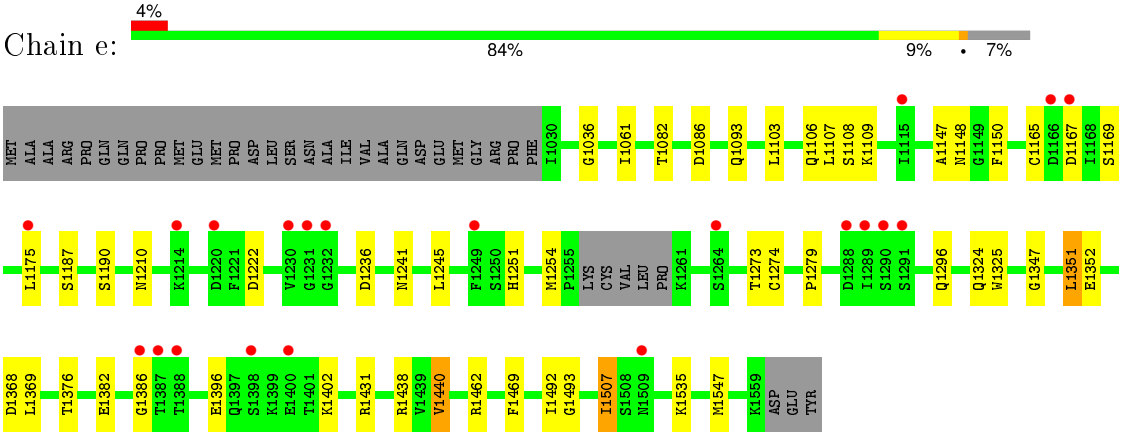
Chain M:





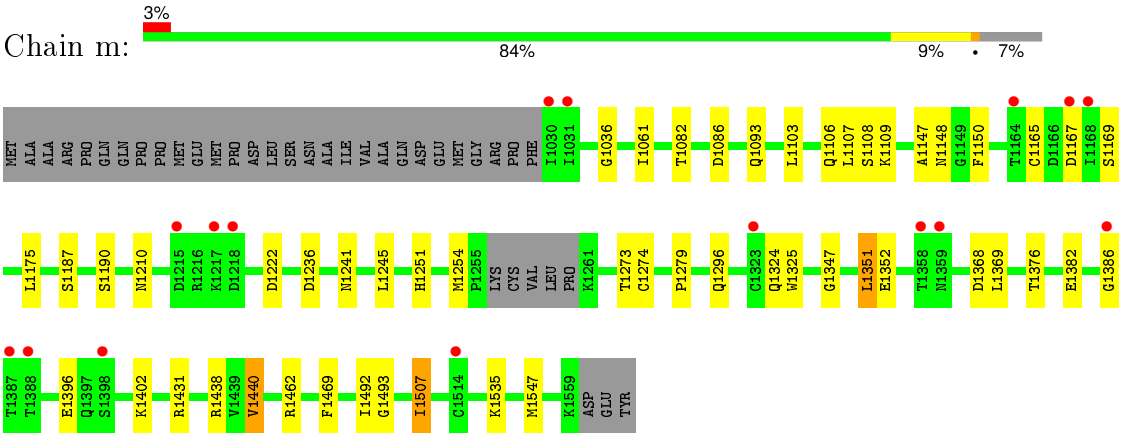
• Molecule 5: T-complex protein 1 subunit epsilon

Chain e:



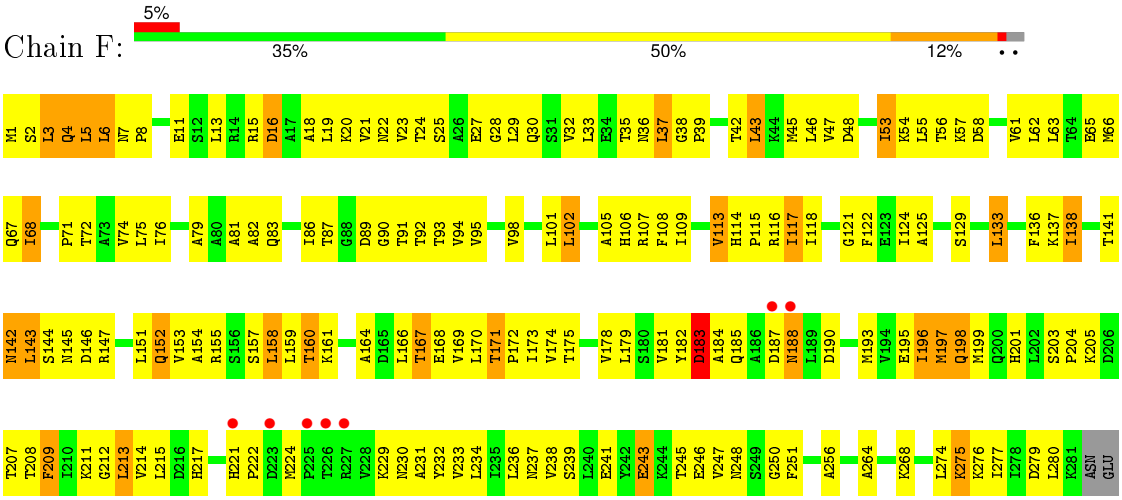
• Molecule 5: T-complex protein 1 subunit epsilon

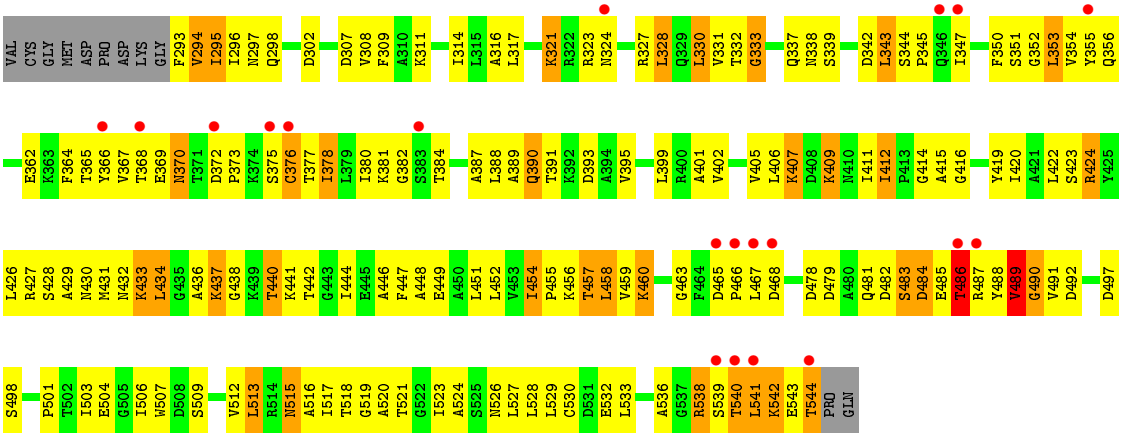
Chain m:



• Molecule 6: T-complex protein 1 subunit zeta

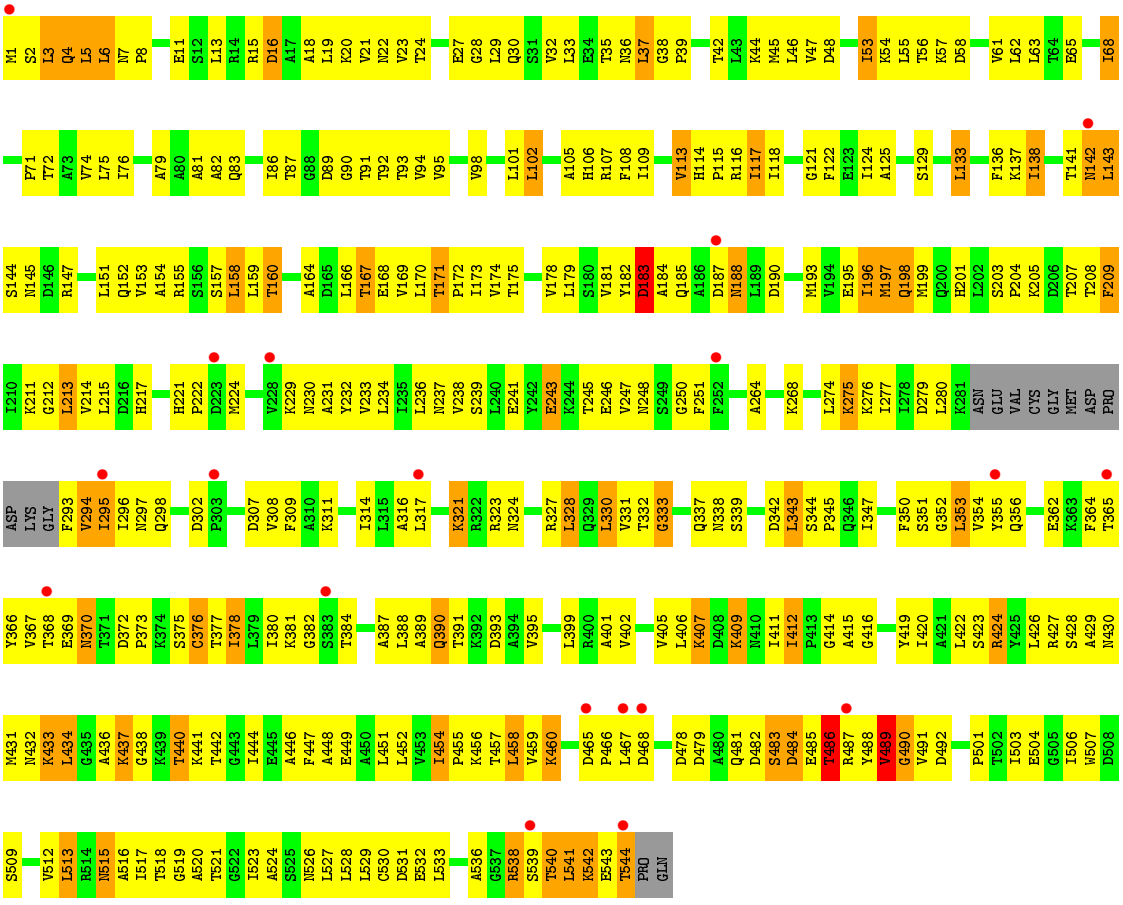
Chain F:





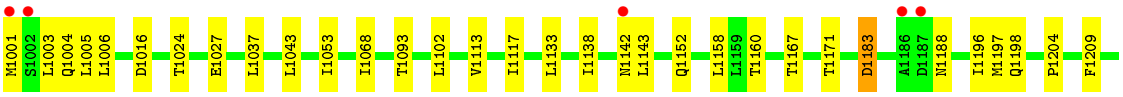
• Molecule 6: T-complex protein 1 subunit zeta

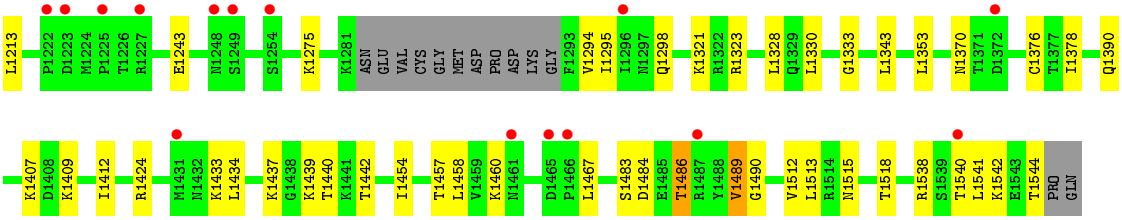
Chain N:



• Molecule 6: T-complex protein 1 subunit zeta

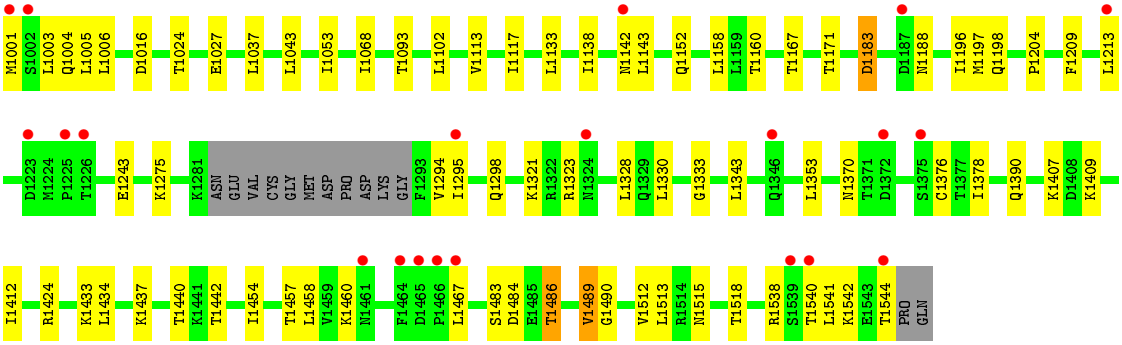
Chain f:





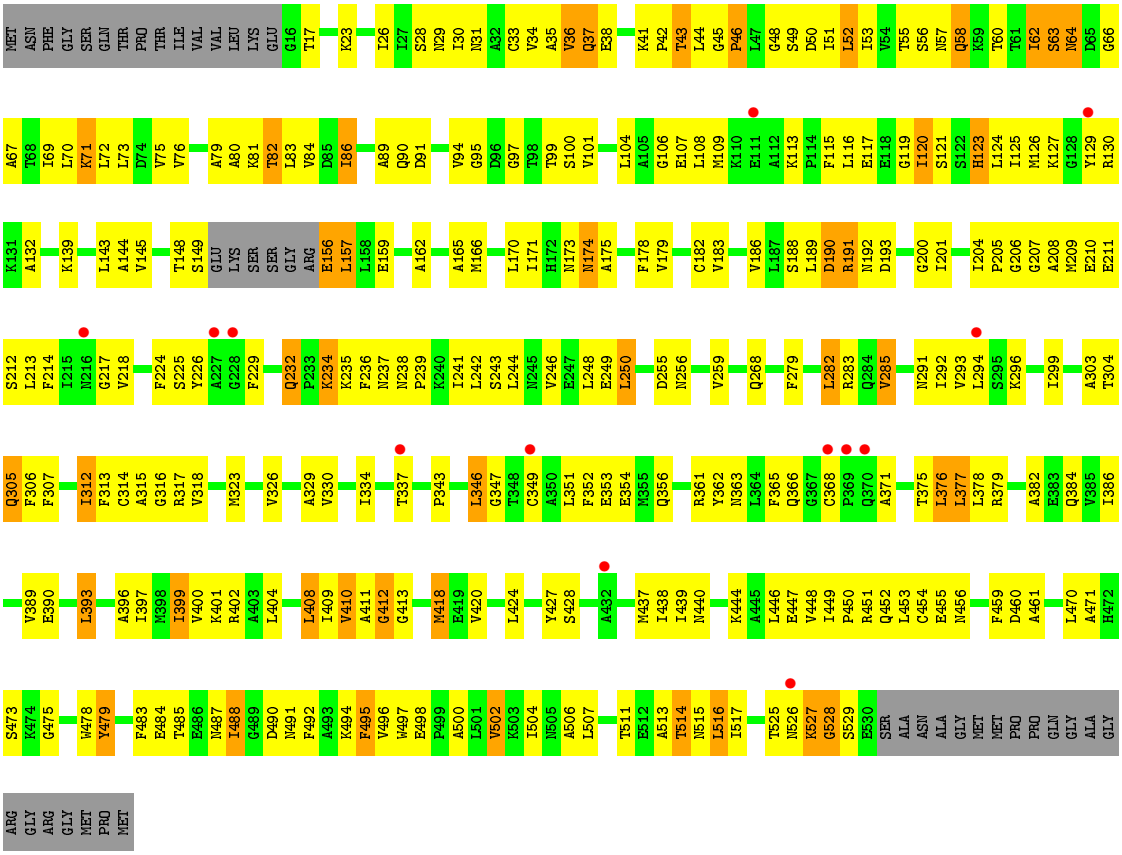
• Molecule 6: T-complex protein 1 subunit zeta

Chain n:



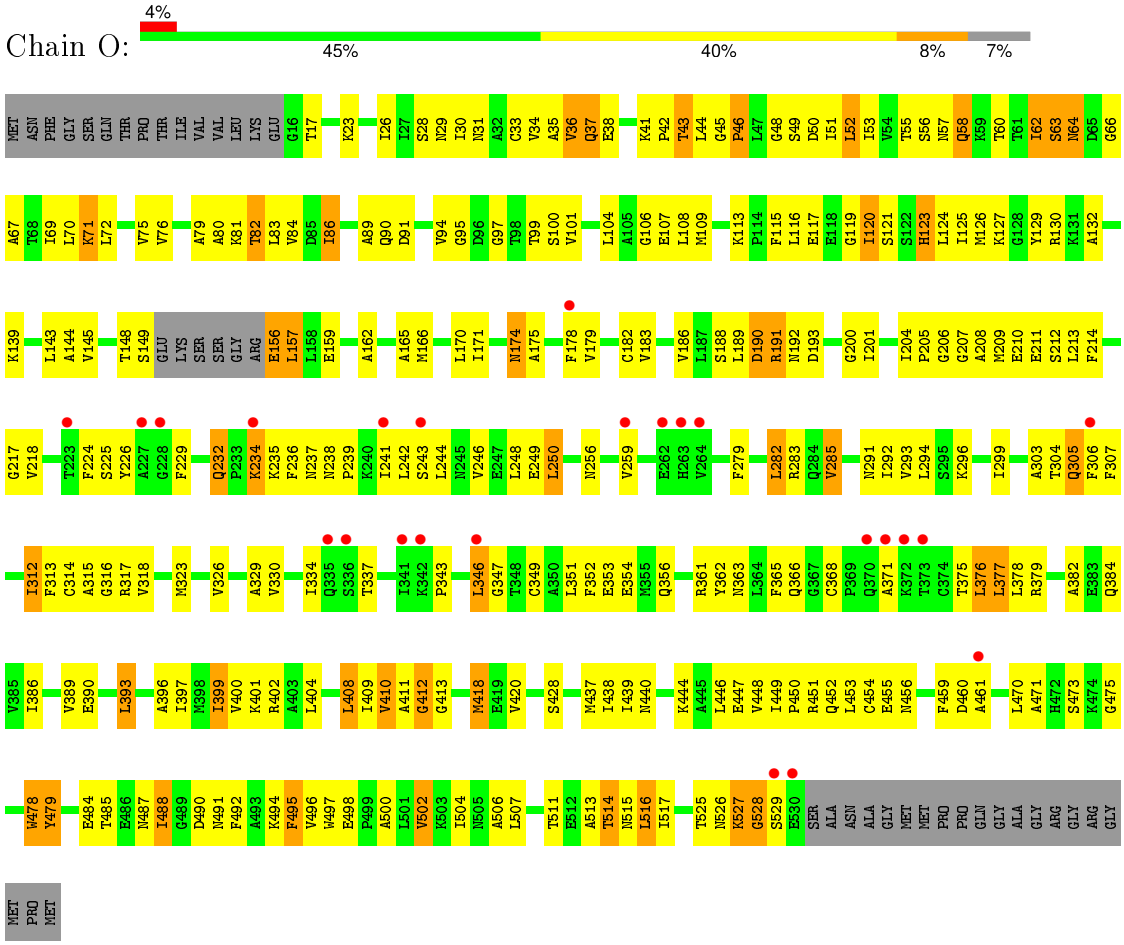
• Molecule 7: T-complex protein 1 subunit eta

Chain G:



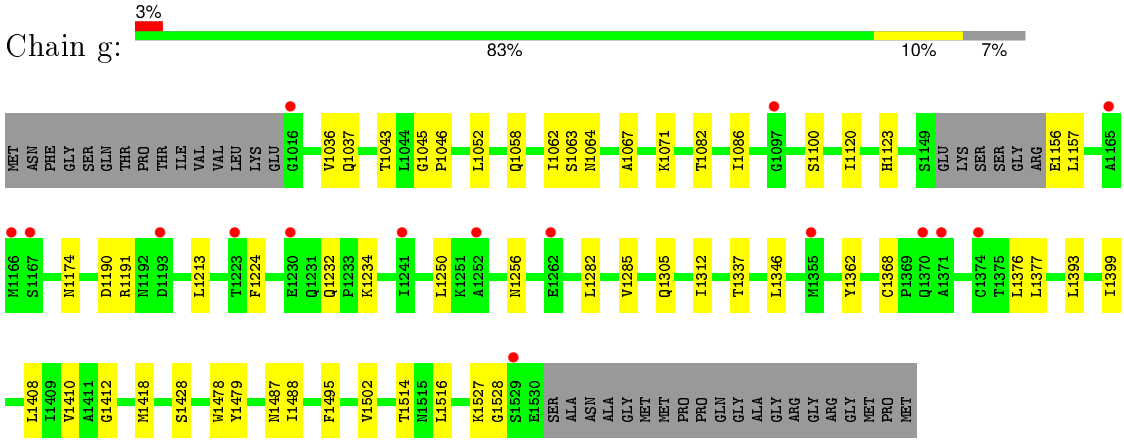
• Molecule 7: T-complex protein 1 subunit eta

Chain O:



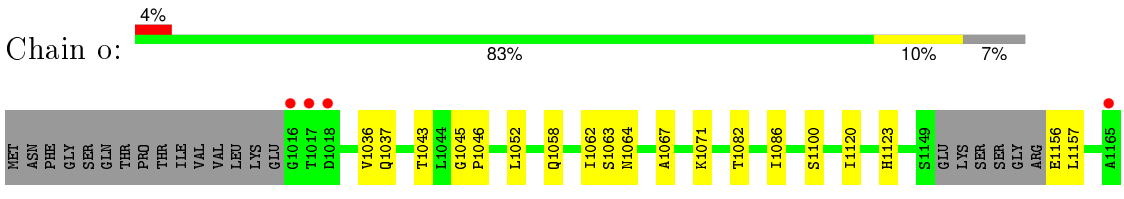
• Molecule 7: T-complex protein 1 subunit eta

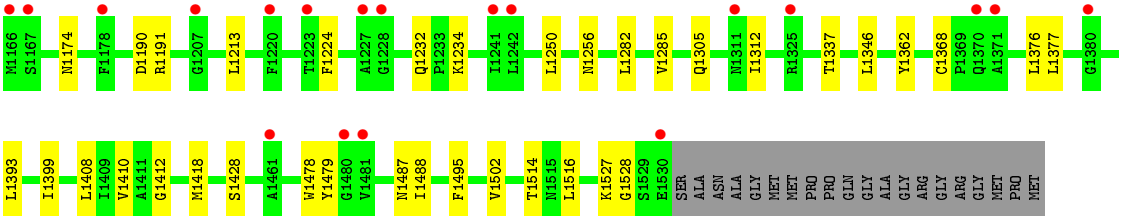
Chain g:



• Molecule 7: T-complex protein 1 subunit eta

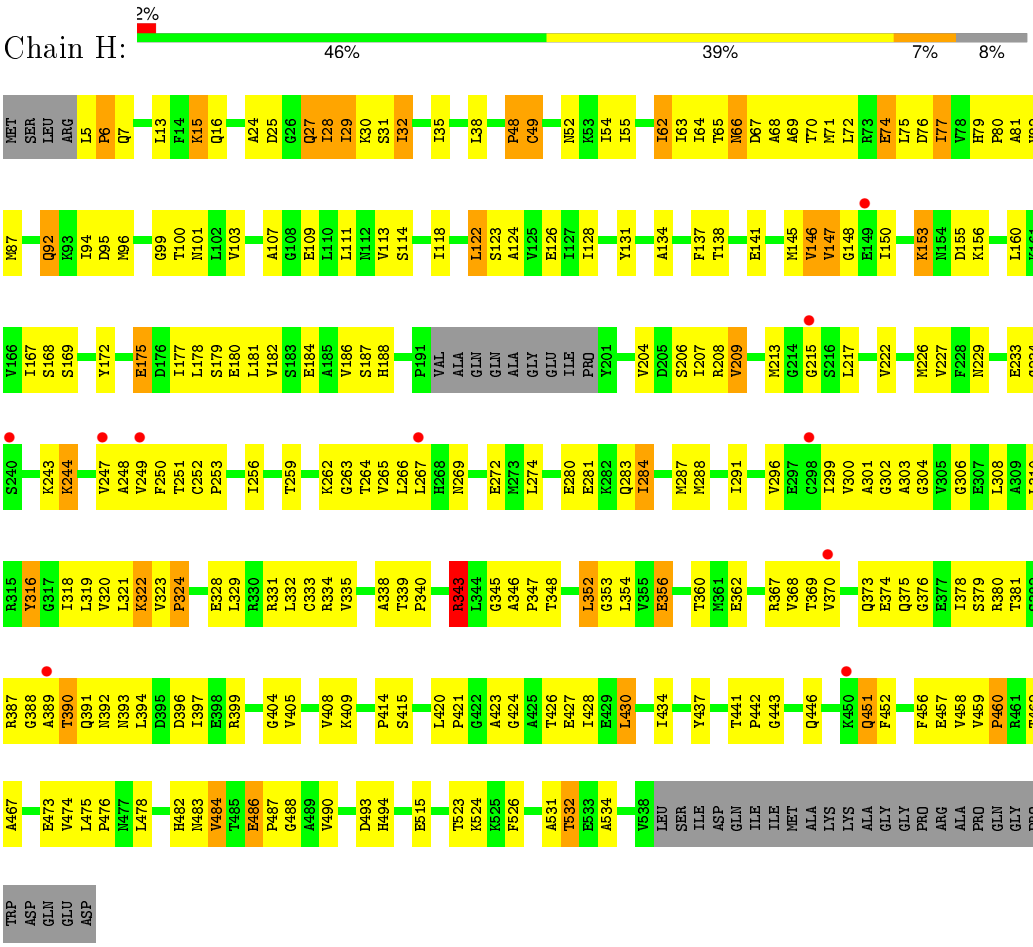
Chain o:





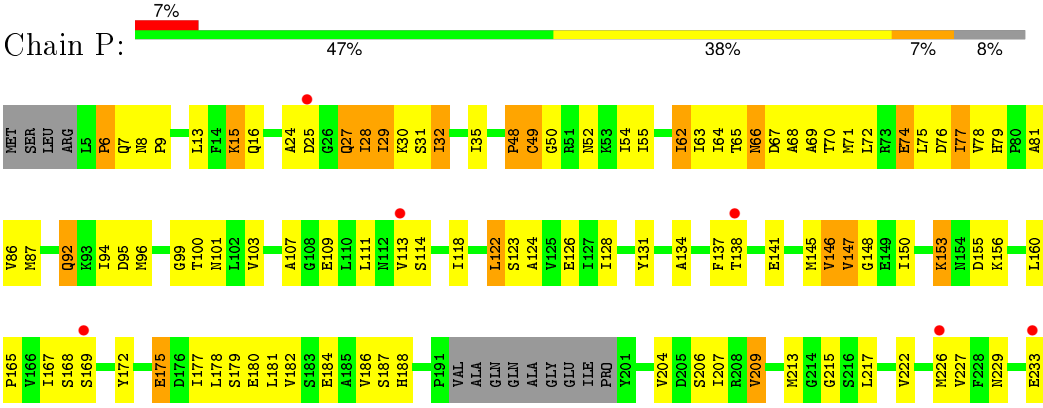
• Molecule 8: T-complex protein 1 subunit theta

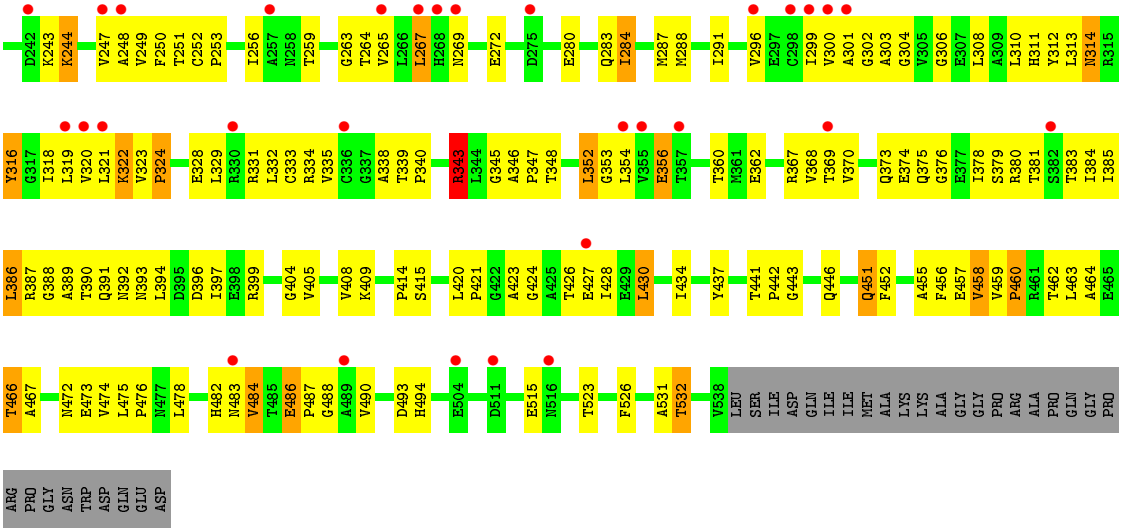
Chain H:



• Molecule 8: T-complex protein 1 subunit theta

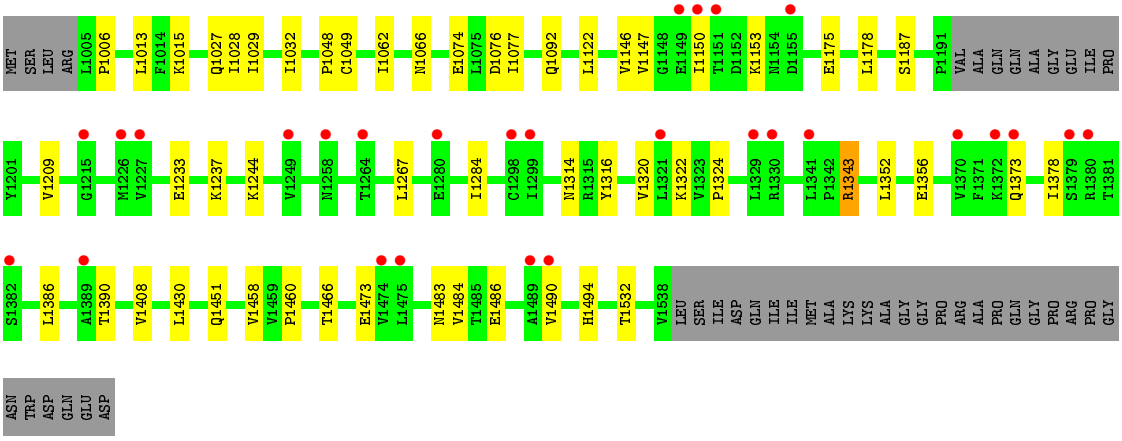
Chain P:





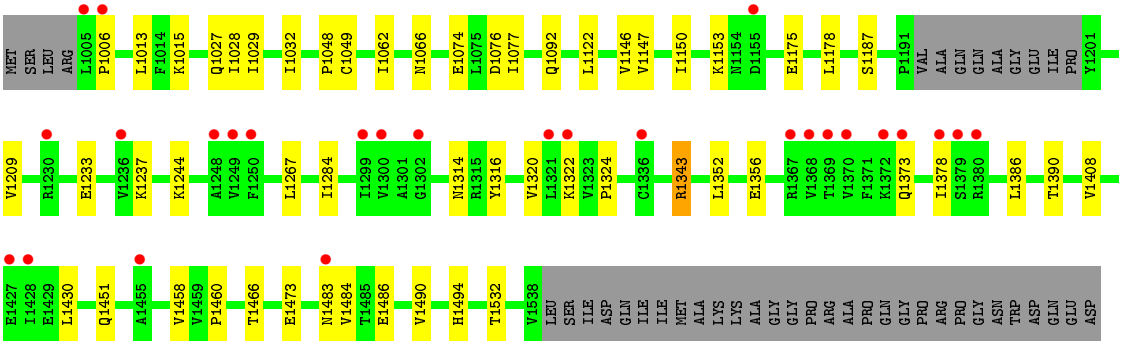
• Molecule 8: T-complex protein 1 subunit theta

Chain h:



• Molecule 8: T-complex protein 1 subunit theta

Chain p:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	89.95 – 3.80 89.95 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (89.95-3.80) 91.2 (89.95-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.307 , 0.344 0.318 , 0.349	Depositor DCC
R_{free} test set	10483 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	112.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 193.3	EDS
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 209673 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	111235	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BEF, SO4, ADP

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	0.23	0/3515	0.47	1/4835 (0.0%)
1	I	0.23	0/3515	0.47	1/4835 (0.0%)
1	a	0.23	0/3515	0.47	1/4835 (0.0%)
1	i	0.23	0/3515	0.47	1/4835 (0.0%)
2	B	0.26	0/3480	0.49	0/4754
2	J	0.26	0/3480	0.49	0/4754
2	b	0.26	0/3481	0.49	0/4755
2	j	0.26	0/3478	0.49	0/4751
3	C	0.23	0/3421	0.46	0/4689
3	K	0.23	0/3422	0.46	0/4690
3	c	0.23	0/3424	0.46	0/4693
3	k	0.23	0/3424	0.46	0/4693
4	D	0.23	0/3421	0.46	2/4683 (0.0%)
4	L	0.23	0/3421	0.45	1/4683 (0.0%)
4	d	0.23	0/3421	0.45	1/4683 (0.0%)
4	l	0.23	0/3421	0.45	1/4683 (0.0%)
5	E	0.23	0/3466	0.46	0/4739
5	M	0.23	0/3466	0.46	0/4739
5	e	0.23	0/3466	0.46	0/4739
5	m	0.23	0/3466	0.46	0/4739
6	F	0.26	0/3663	0.52	1/5008 (0.0%)
6	N	0.26	0/3660	0.52	1/5004 (0.0%)
6	f	0.26	0/3665	0.52	1/5009 (0.0%)
6	n	0.26	0/3661	0.52	1/5005 (0.0%)
7	G	0.23	0/3342	0.46	0/4578
7	O	0.23	0/3339	0.45	0/4574
7	g	0.23	0/3339	0.45	0/4574
7	o	0.23	0/3339	0.45	0/4574
8	H	0.22	0/3522	0.42	0/4825
8	P	0.22	0/3522	0.42	0/4825
8	h	0.22	0/3519	0.42	0/4820
8	p	0.22	0/3522	0.42	0/4825

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.24	0/111311	0.47	13/152428 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	437	ALA	CB-CA-C	8.54	122.92	110.10
1	i	1437	ALA	CB-CA-C	8.53	122.89	110.10
1	A	437	ALA	CB-CA-C	8.53	122.89	110.10
1	a	1437	ALA	CB-CA-C	8.52	122.88	110.10
4	L	350	VAL	N-CA-C	-6.53	93.36	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3492	0	3026	298	0
1	I	3492	0	3026	291	0
1	a	3492	0	3026	0	0
1	i	3492	0	3026	0	0
2	B	3459	0	3146	476	0
2	J	3459	0	3146	479	0
2	b	3460	0	3148	0	0
2	j	3457	0	3139	0	0
3	C	3392	0	3019	295	0
3	K	3393	0	3022	272	0
3	c	3395	0	3029	0	0
3	k	3395	0	3029	0	0
4	D	3398	0	3010	337	0
4	L	3398	0	3010	315	0
4	d	3398	0	3010	0	0
4	l	3398	0	3010	0	0
5	E	3437	0	2943	285	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	3437	0	2943	289	0
5	e	3437	0	2943	0	0
5	m	3437	0	2943	0	0
6	F	3631	0	3330	640	0
6	N	3628	0	3321	629	0
6	f	3633	0	3333	0	0
6	n	3629	0	3322	0	0
7	G	3317	0	2920	382	0
7	O	3314	0	2911	375	0
7	g	3314	0	2911	0	0
7	o	3314	0	2911	0	0
8	H	3487	0	3109	296	0
8	P	3487	0	3109	273	0
8	h	3485	0	3103	0	0
8	p	3487	0	3109	0	0
9	A	27	0	11	3	0
9	B	27	0	11	8	0
9	C	27	0	12	7	0
9	D	27	0	11	8	0
9	E	27	0	11	2	0
9	F	27	0	11	6	0
9	G	27	0	11	5	0
9	H	27	0	12	3	0
9	J	27	0	11	5	0
9	L	27	0	11	7	0
9	M	27	0	11	6	0
9	N	27	0	11	6	0
9	P	27	0	12	5	0
9	a	27	0	11	0	0
9	b	27	0	11	0	0
9	e	27	0	12	0	0
9	f	27	0	11	0	0
9	g	27	0	11	0	0
9	h	27	0	12	0	0
9	k	27	0	11	0	0
9	l	27	0	11	0	0
9	m	27	0	11	0	0
9	n	27	0	11	0	0
9	p	27	0	12	0	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
10	C	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	4	0	0	0	0
10	E	4	0	0	0	0
10	F	4	0	0	2	0
10	G	4	0	0	0	0
10	H	4	0	0	0	0
10	J	4	0	0	0	0
10	L	4	0	0	1	0
10	M	4	0	0	0	0
10	N	4	0	0	3	0
10	P	4	0	0	0	0
10	a	4	0	0	0	0
10	b	4	0	0	0	0
10	e	4	0	0	0	0
10	f	4	0	0	0	0
10	g	4	0	0	0	0
10	h	4	0	0	0	0
10	k	4	0	0	0	0
10	l	4	0	0	0	0
10	m	4	0	0	0	0
10	n	4	0	0	0	0
10	p	4	0	0	0	0
11	I	5	0	0	0	0
11	K	5	0	0	0	0
11	O	5	0	0	0	0
11	c	5	0	0	0	0
11	d	5	0	0	0	0
11	i	5	0	0	0	0
11	j	5	0	0	0	0
11	o	5	0	0	0	0
12	B	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	M	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	m	1	0	0	0	0
All	All	111235	0	98253	5533	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 53.

The worst 5 of 5533 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:B:4:GLN:HA	2:B:5:ILE:CG1	1.37	1.53
2:J:4:GLN:HA	2:J:5:ILE:CG1	1.37	1.48
6:N:36:ASN:HB3	6:N:57:LYS:NZ	1.28	1.46
6:F:151:LEU:CD1	6:F:175:THR:CG2	1.90	1.46
6:N:151:LEU:CD1	6:N:175:THR:CG2	1.90	1.46

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	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
1	I	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
1	a	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
1	i	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	4	42
2	B	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	3	32
2	J	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	3	32
2	b	509/527 (97%)	417 (82%)	68 (13%)	24 (5%)	3	33
2	j	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	3	32
3	C	508/590 (86%)	420 (83%)	68 (13%)	20 (4%)	4	38
3	K	508/590 (86%)	421 (83%)	67 (13%)	20 (4%)	4	38
3	c	508/590 (86%)	419 (82%)	70 (14%)	19 (4%)	4	40
3	k	508/590 (86%)	420 (83%)	68 (13%)	20 (4%)	4	38
4	D	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51
4	L	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51
4	d	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51
4	l	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	8	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	4	41
5	M	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	4	41
5	e	521/562 (93%)	442 (85%)	60 (12%)	19 (4%)	4	41
5	m	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	4	41
6	F	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
6	N	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
6	f	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
6	n	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	5	43
7	G	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
7	O	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
7	g	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
7	o	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	3	36
8	H	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
8	P	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
8	h	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
8	p	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	3	34
All	All	16604/17720 (94%)	13767 (83%)	2207 (13%)	630 (4%)	4	39

5 of 630 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	ILE
2	B	165	ILE
2	B	184	LEU
2	B	185	LYS
2	B	307	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	301/471 (64%)	274 (91%)	27 (9%)	12 49
1	I	301/471 (64%)	274 (91%)	27 (9%)	12 49
1	a	301/471 (64%)	274 (91%)	27 (9%)	12 49
1	i	301/471 (64%)	274 (91%)	27 (9%)	12 49
2	B	320/441 (73%)	263 (82%)	57 (18%)	2 17
2	J	320/441 (73%)	263 (82%)	57 (18%)	2 17
2	b	320/441 (73%)	262 (82%)	58 (18%)	2 16
2	j	319/441 (72%)	262 (82%)	57 (18%)	2 16
3	C	295/497 (59%)	268 (91%)	27 (9%)	11 48
3	K	296/497 (60%)	269 (91%)	27 (9%)	12 48
3	c	297/497 (60%)	270 (91%)	27 (9%)	12 48
3	k	297/497 (60%)	270 (91%)	27 (9%)	12 48
4	D	290/454 (64%)	261 (90%)	29 (10%)	9 43
4	L	290/454 (64%)	261 (90%)	29 (10%)	9 43
4	d	290/454 (64%)	261 (90%)	29 (10%)	9 43
4	l	290/454 (64%)	261 (90%)	29 (10%)	9 43
5	E	293/483 (61%)	257 (88%)	36 (12%)	6 34
5	M	293/483 (61%)	257 (88%)	36 (12%)	6 34
5	e	293/483 (61%)	257 (88%)	36 (12%)	6 34
5	m	293/483 (61%)	257 (88%)	36 (12%)	6 34
6	F	334/463 (72%)	273 (82%)	61 (18%)	2 15
6	N	333/463 (72%)	273 (82%)	60 (18%)	2 16
6	f	334/463 (72%)	272 (81%)	62 (19%)	2 14
6	n	333/463 (72%)	272 (82%)	61 (18%)	2 15
7	G	275/454 (61%)	241 (88%)	34 (12%)	6 33
7	O	274/454 (60%)	240 (88%)	34 (12%)	6 33
7	g	274/454 (60%)	240 (88%)	34 (12%)	6 33
7	o	274/454 (60%)	240 (88%)	34 (12%)	6 33
8	H	307/473 (65%)	276 (90%)	31 (10%)	9 43
8	P	307/473 (65%)	276 (90%)	31 (10%)	9 43
8	h	306/473 (65%)	275 (90%)	31 (10%)	9 43
8	p	307/473 (65%)	276 (90%)	31 (10%)	9 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9658/14944 (65%)	8449 (88%)	1209 (12%)	6 33

5 of 1209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	O	86	ILE
2	b	1427	SER
6	n	1370	ASN
7	O	377	LEU
1	a	1187	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 306 such sidechains are listed below:

Mol	Chain	Res	Type
7	O	58	GLN
2	b	1271	ASN
6	n	1104	GLN
7	O	491	ASN
1	a	1121	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

56 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	ADP	A	601	10	22,29,29	2.06	8 (36%)	27,45,45	2.99	10 (37%)
10	BEF	A	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	B	601	10	22,29,29	2.08	9 (40%)	27,45,45	2.96	9 (33%)
10	BEF	B	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	C	1101	-	22,29,29	2.01	8 (36%)	27,45,45	2.79	5 (18%)
10	BEF	C	1102	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	D	601	-	22,29,29	1.99	8 (36%)	27,45,45	2.85	8 (29%)
10	BEF	D	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	E	601	10	22,29,29	2.07	9 (40%)	27,45,45	3.00	8 (29%)
10	BEF	E	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	F	601	-	22,29,29	2.06	9 (40%)	27,45,45	2.87	9 (33%)
10	BEF	F	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	G	601	-	22,29,29	2.09	8 (36%)	27,45,45	3.03	10 (37%)
10	BEF	G	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	H	601	-	22,29,29	2.02	8 (36%)	27,45,45	2.89	7 (25%)
10	BEF	H	602	-	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	I	600	-	4,4,4	0.18	0	6,6,6	0.12	0
9	ADP	J	601	10	22,29,29	2.03	9 (40%)	27,45,45	3.12	11 (40%)
10	BEF	J	602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	K	1101	-	4,4,4	0.21	0	6,6,6	0.17	0
9	ADP	L	601	-	22,29,29	2.02	8 (36%)	27,45,45	2.80	8 (29%)
10	BEF	L	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	M	601	-	22,29,29	2.00	9 (40%)	27,45,45	2.92	8 (29%)
10	BEF	M	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	N	601	10	22,29,29	2.05	8 (36%)	27,45,45	2.94	10 (37%)
10	BEF	N	602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	O	600	-	4,4,4	0.10	0	6,6,6	0.12	0
9	ADP	P	601	-	22,29,29	2.02	8 (36%)	27,45,45	2.90	11 (40%)
10	BEF	P	602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	a	1601	-	22,29,29	2.02	8 (36%)	27,45,45	3.00	10 (37%)
10	BEF	a	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	b	1601	10	22,29,29	2.03	9 (40%)	27,45,45	2.85	11 (40%)
10	BEF	b	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	c	2101	-	4,4,4	0.20	0	6,6,6	0.18	0
11	SO4	d	1600	-	4,4,4	0.18	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	ADP	e	1601	-	22,29,29	2.03	8 (36%)	27,45,45	2.84	8 (29%)
10	BEF	e	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	f	1601	-	22,29,29	2.05	8 (36%)	27,45,45	3.04	10 (37%)
10	BEF	f	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	g	1601	-	22,29,29	2.06	8 (36%)	27,45,45	2.85	9 (33%)
10	BEF	g	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	h	1601	10	22,29,29	2.04	9 (40%)	27,45,45	2.72	9 (33%)
10	BEF	h	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	i	1600	-	4,4,4	0.18	0	6,6,6	0.29	0
11	SO4	j	1600	-	4,4,4	0.21	0	6,6,6	0.15	0
9	ADP	k	2101	10	22,29,29	2.03	9 (40%)	27,45,45	3.04	9 (33%)
10	BEF	k	2102	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	l	1601	10	22,29,29	2.05	8 (36%)	27,45,45	2.94	9 (33%)
10	BEF	l	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	m	1601	-	22,29,29	2.06	9 (40%)	27,45,45	2.83	8 (29%)
10	BEF	m	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	n	1601	-	22,29,29	2.01	9 (40%)	27,45,45	2.86	10 (37%)
10	BEF	n	1602	-	0,3,3	0.00	-	0,3,3	0.00	-
11	SO4	o	1600	-	4,4,4	0.23	0	6,6,6	0.13	0
9	ADP	p	1601	10	22,29,29	2.07	8 (36%)	27,45,45	2.85	11 (40%)
10	BEF	p	1602	9	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	A	601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	A	602	9	-	0/0/0/0	0/0/0/0
9	ADP	B	601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	B	602	9	-	0/0/0/0	0/0/0/0
9	ADP	C	1101	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	C	1102	-	-	0/0/0/0	0/0/0/0
9	ADP	D	601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	D	602	-	-	0/0/0/0	0/0/0/0
9	ADP	E	601	10	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	E	602	9	-	0/0/0/0	0/0/0/0
9	ADP	F	601	-	-	0/12/32/32	0/3/3/3
10	BEF	F	602	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	G	601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	G	602	-	-	0/0/0/0	0/0/0/0
9	ADP	H	601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	H	602	-	-	0/0/0/0	0/0/0/0
11	SO4	I	600	-	-	0/0/0/0	0/0/0/0
9	ADP	J	601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	J	602	9	-	0/0/0/0	0/0/0/0
11	SO4	K	1101	-	-	0/0/0/0	0/0/0/0
9	ADP	L	601	-	-	0/12/32/32	0/3/3/3
10	BEF	L	602	-	-	0/0/0/0	0/0/0/0
9	ADP	M	601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	M	602	-	-	0/0/0/0	0/0/0/0
9	ADP	N	601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	N	602	9	-	0/0/0/0	0/0/0/0
11	SO4	O	600	-	-	0/0/0/0	0/0/0/0
9	ADP	P	601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	P	602	-	-	0/0/0/0	0/0/0/0
9	ADP	a	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	a	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	b	1601	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	b	1602	9	-	0/0/0/0	0/0/0/0
11	SO4	c	2101	-	-	0/0/0/0	0/0/0/0
11	SO4	d	1600	-	-	0/0/0/0	0/0/0/0
9	ADP	e	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	e	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	f	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	f	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	g	1601	-	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	g	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	h	1601	10	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	h	1602	9	-	0/0/0/0	0/0/0/0
11	SO4	i	1600	-	-	0/0/0/0	0/0/0/0
11	SO4	j	1600	-	-	0/0/0/0	0/0/0/0
9	ADP	k	2101	10	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	k	2102	9	-	0/0/0/0	0/0/0/0
9	ADP	l	1601	10	-	0/12/32/32	0/3/3/3
10	BEF	l	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	m	1601	-	2/2/6/6	0/12/32/32	0/3/3/3
10	BEF	m	1602	-	-	0/0/0/0	0/0/0/0
9	ADP	n	1601	-	1/1/6/6	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BEF	n	1602	-	-	0/0/0/0	0/0/0/0
11	SO4	o	1600	-	-	0/0/0/0	0/0/0/0
9	ADP	p	1601	10	1/1/6/6	0/12/32/32	0/3/3/3
10	BEF	p	1602	9	-	0/0/0/0	0/0/0/0

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	601	ADP	C5-C4	-2.68	1.34	1.40
9	F	601	ADP	C5-C4	-2.66	1.34	1.40
9	e	1601	ADP	C5-C4	-2.60	1.34	1.40
9	g	1601	ADP	C5-C4	-2.60	1.34	1.40
9	a	1601	ADP	C5-C4	-2.56	1.34	1.40

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	601	ADP	N3-C2-N1	-12.45	119.36	128.89
9	H	601	ADP	N3-C2-N1	-12.17	119.58	128.89
9	l	1601	ADP	N3-C2-N1	-11.93	119.76	128.89
9	a	1601	ADP	N3-C2-N1	-11.81	119.86	128.89
9	P	601	ADP	N3-C2-N1	-11.67	119.96	128.89

5 of 34 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	J	601	ADP	C4'
9	J	601	ADP	C3'
9	a	1601	ADP	C4'
9	a	1601	ADP	C3'
9	P	601	ADP	C4'

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	601	ADP	3	0
9	B	601	ADP	8	0
9	C	1101	ADP	7	0
10	C	1102	BEF	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	601	ADP	8	0
9	E	601	ADP	2	0
9	F	601	ADP	6	0
10	F	602	BEF	2	0
9	G	601	ADP	5	0
9	H	601	ADP	3	0
9	J	601	ADP	5	0
9	L	601	ADP	7	0
10	L	602	BEF	1	0
9	M	601	ADP	6	0
9	N	601	ADP	6	0
10	N	602	BEF	3	0
9	P	601	ADP	5	0

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^{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	544/559 (97%)	0.03	13 (2%) 62 46	72, 134, 206, 254	0
1	I	544/559 (97%)	0.05	26 (4%) 34 22	72, 134, 206, 254	0
1	a	544/559 (97%)	-0.06	15 (2%) 56 40	72, 134, 206, 254	0
1	i	544/559 (97%)	-0.03	14 (2%) 59 43	72, 134, 206, 254	0
2	B	513/527 (97%)	-0.08	5 (0%) 84 72	47, 120, 192, 236	0
2	J	513/527 (97%)	0.08	19 (3%) 45 30	47, 120, 192, 236	0
2	b	513/527 (97%)	-0.07	10 (1%) 70 54	47, 120, 192, 236	0
2	j	513/527 (97%)	-0.06	7 (1%) 78 63	47, 120, 192, 236	0
3	C	514/590 (87%)	0.09	10 (1%) 70 54	73, 141, 205, 295	0
3	K	514/590 (87%)	0.04	19 (3%) 45 30	73, 141, 205, 295	0
3	c	514/590 (87%)	0.06	18 (3%) 48 32	73, 141, 205, 295	0
3	k	514/590 (87%)	-0.05	11 (2%) 67 51	73, 141, 205, 295	0
4	D	522/528 (98%)	0.03	15 (2%) 55 38	70, 149, 232, 297	0
4	L	522/528 (98%)	0.10	27 (5%) 31 21	70, 149, 232, 297	0
4	d	522/528 (98%)	0.04	15 (2%) 55 38	70, 149, 232, 297	0
4	l	522/528 (98%)	0.12	22 (4%) 40 26	70, 149, 232, 297	0
5	E	525/562 (93%)	0.08	17 (3%) 51 35	56, 138, 238, 297	0
5	M	525/562 (93%)	0.25	34 (6%) 22 13	56, 138, 238, 297	0
5	e	525/562 (93%)	0.05	21 (4%) 42 28	56, 138, 238, 297	0
5	m	525/562 (93%)	-0.03	16 (3%) 54 37	56, 138, 238, 297	0
6	F	533/546 (97%)	0.13	27 (5%) 32 21	42, 116, 214, 301	0
6	N	533/546 (97%)	0.08	19 (3%) 46 32	42, 116, 214, 301	0
6	f	533/546 (97%)	0.10	20 (3%) 44 30	42, 116, 214, 301	0
6	n	533/546 (97%)	0.08	21 (3%) 43 29	42, 116, 214, 301	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
7	G	509/550 (92%)	0.06	13 (2%)	59	43	65, 136, 207, 264	0
7	O	509/550 (92%)	0.16	24 (4%)	35	23	65, 136, 207, 264	0
7	g	509/550 (92%)	-0.02	16 (3%)	52	36	65, 136, 207, 264	0
7	o	509/550 (92%)	0.12	23 (4%)	37	24	65, 136, 207, 264	0
8	H	525/568 (92%)	0.04	11 (2%)	67	51	70, 148, 236, 294	0
8	P	525/568 (92%)	0.29	38 (7%)	18	11	70, 148, 236, 294	0
8	h	525/568 (92%)	0.18	28 (5%)	30	20	70, 148, 236, 294	0
8	p	525/568 (92%)	0.14	27 (5%)	32	21	70, 148, 236, 294	0
All	All	16740/17720 (94%)	0.06	601 (3%)	46	32	42, 136, 217, 301	0

The worst 5 of 601 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	1387	THR	13.8
5	M	387	THR	12.1
7	o	1228	GLY	11.4
5	m	1387	THR	10.0
6	n	1539	SER	8.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
10	BEF	B	602	4/4	0.90	0.33	3.98	210,215,215,215	0
10	BEF	E	602	4/4	0.87	0.43	3.63	240,241,242,244	0
10	BEF	G	602	4/4	0.89	0.42	2.91	236,237,238,239	0
11	SO4	d	1600	5/5	0.95	0.29	1.74	106,109,115,118	0
11	SO4	c	2101	5/5	0.95	0.28	1.46	82,98,107,111	0
10	BEF	J	602	4/4	0.81	0.29	1.31	235,236,240,246	0
11	SO4	I	600	5/5	0.94	0.28	1.06	98,103,110,113	0
10	BEF	m	1602	4/4	0.95	0.26	0.96	185,193,195,196	0
10	BEF	A	602	4/4	0.90	0.37	0.87	246,247,249,251	0
9	ADP	A	601	27/27	0.90	0.35	0.77	46,110,243,330	0
10	BEF	N	602	4/4	0.95	0.31	0.74	112,120,121,122	0
11	SO4	j	1600	5/5	0.92	0.29	0.70	79,96,98,100	0
10	BEF	a	1602	4/4	0.85	0.25	0.64	235,239,240,241	0
9	ADP	h	1601	27/27	0.94	0.33	0.63	40,139,153,188	0
10	BEF	F	602	4/4	0.97	0.27	0.61	157,163,163,171	0
11	SO4	i	1600	5/5	0.96	0.28	0.51	91,94,103,116	0
9	ADP	F	601	27/27	0.95	0.30	0.50	11,105,323,481	0
9	ADP	l	1601	27/27	0.87	0.29	0.40	62,105,189,226	0
11	SO4	K	1101	5/5	0.96	0.35	0.34	84,89,97,102	0
9	ADP	B	601	27/27	0.90	0.27	0.29	62,105,202,218	0
9	ADP	E	601	27/27	0.91	0.32	0.23	11,102,242,288	0
9	ADP	f	1601	27/27	0.90	0.28	0.14	13,50,316,499	0
10	BEF	f	1602	4/4	0.95	0.23	0.09	167,170,171,173	0
9	ADP	L	601	27/27	0.90	0.24	-0.01	102,157,212,241	0
10	BEF	e	1602	4/4	0.96	0.21	-0.03	201,205,207,207	0
9	ADP	a	1601	27/27	0.92	0.23	-0.10	50,112,239,328	0
9	ADP	N	601	27/27	0.95	0.24	-0.11	11,88,232,484	0
9	ADP	k	2101	27/27	0.95	0.28	-0.15	80,131,164,321	0
9	ADP	m	1601	27/27	0.90	0.24	-0.19	13,87,195,273	0
9	ADP	n	1601	27/27	0.93	0.26	-0.19	27,94,337,491	0
9	ADP	p	1601	27/27	0.94	0.21	-0.35	11,114,136,239	0
9	ADP	H	601	27/27	0.94	0.24	-0.35	11,112,145,153	0
9	ADP	C	1101	27/27	0.92	0.28	-0.40	38,135,163,237	0
9	ADP	J	601	27/27	0.93	0.24	-0.43	74,85,241,279	0
10	BEF	n	1602	4/4	0.97	0.23	-0.48	163,167,167,173	0
11	SO4	O	600	5/5	0.95	0.27	-0.49	78,79,92,100	0
9	ADP	e	1601	27/27	0.93	0.20	-0.54	30,116,232,274	0
9	ADP	M	601	27/27	0.87	0.26	-0.61	43,113,256,333	0
9	ADP	G	601	27/27	0.92	0.21	-0.65	12,133,240,248	0
9	ADP	P	601	27/27	0.94	0.25	-0.69	73,153,161,164	0
10	BEF	C	1102	4/4	0.91	0.21	-0.69	104,105,105,120	0
10	BEF	b	1602	4/4	0.91	0.19	-0.71	154,158,161,163	0
10	BEF	M	602	4/4	0.78	0.23	-0.72	152,158,161,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	ADP	b	1601	27/27	0.95	0.20	-0.75	44,69,220,243	0
9	ADP	g	1601	27/27	0.94	0.19	-0.78	26,159,211,215	0
11	SO4	o	1600	5/5	0.95	0.23	-0.79	107,107,115,117	0
10	BEF	g	1602	4/4	0.97	0.18	-0.85	162,165,165,166	0
9	ADP	D	601	27/27	0.94	0.20	-1.06	41,92,238,264	0
10	BEF	p	1602	4/4	0.97	0.13	-1.30	84,99,102,108	0
10	BEF	P	602	4/4	0.99	0.12	-1.78	158,158,158,162	0
10	BEF	H	602	4/4	0.99	0.11	-1.93	101,103,104,110	0
10	BEF	h	1602	4/4	0.98	0.14	-2.49	85,93,93,106	0
10	BEF	k	2102	4/4	0.94	0.09	-2.80	68,69,80,82	0
10	BEF	D	602	4/4	0.97	0.11	-3.16	81,84,91,92	0
10	BEF	l	1602	4/4	0.96	0.13	-	28,61,73,75	0
10	BEF	L	602	4/4	0.93	0.18	-	172,177,177,180	0

6.5 Other polymers

There are no such residues in this entry.