wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:55 PM GMT

PDB ID	:	4V8R
Title	:	The crystal structures of the eukaryotic chaperonin CCT reveal its functional partitioning
Authors	:	Kalisman, N.; Schroder, G.F.; Levitt, M.
Deposited on	:	2012-03-28
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:

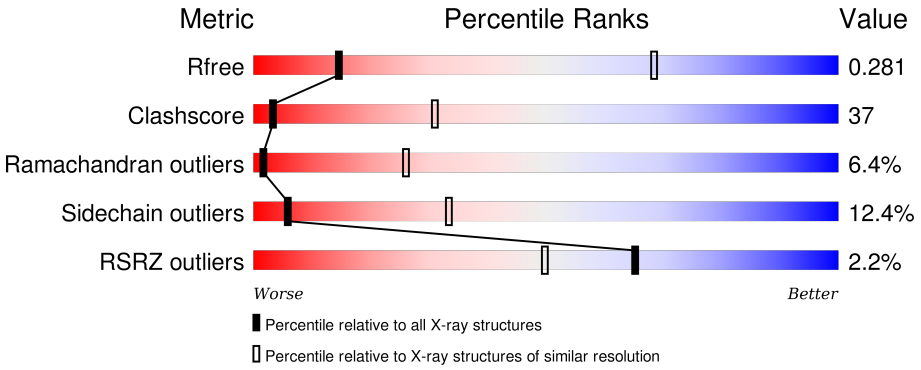
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	AA	559	% 33% 53% 10%
1	Aa	559	% 79% 17%
1	BA	559	% 33% 53% 10%
1	Ba	559	3% 79% 17%
2	AB	527	% 33% 52% 12%

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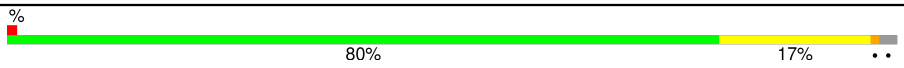
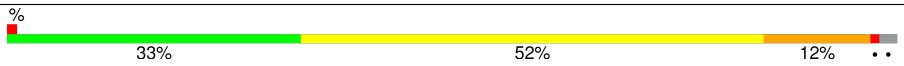
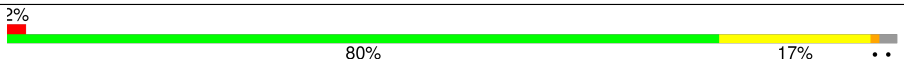
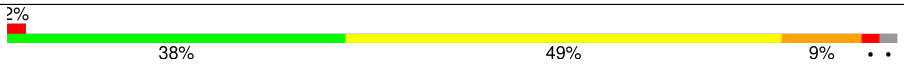
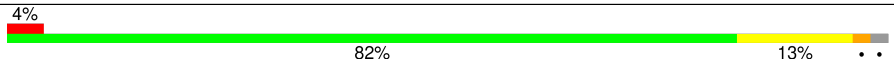
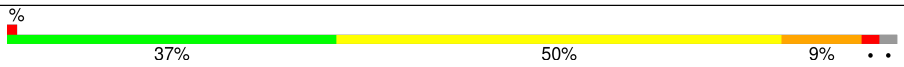
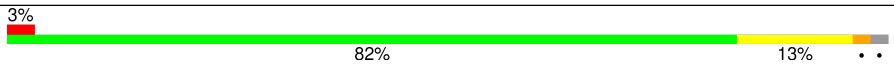
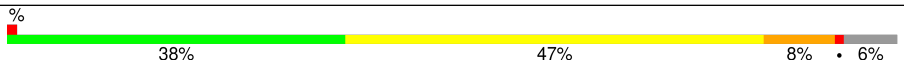
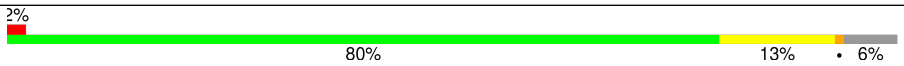
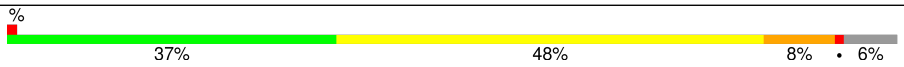
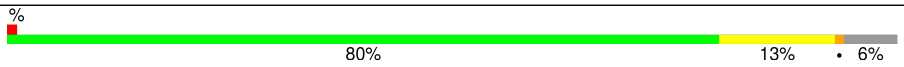
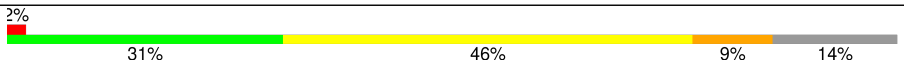
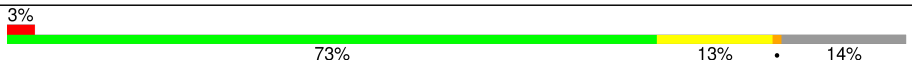
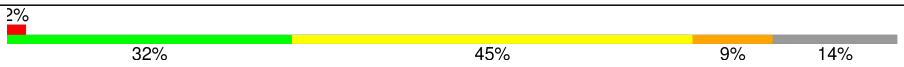
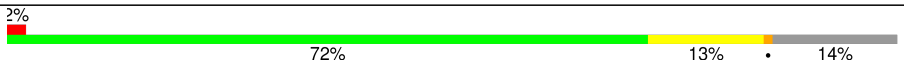
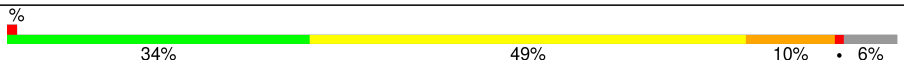
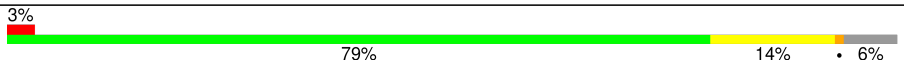
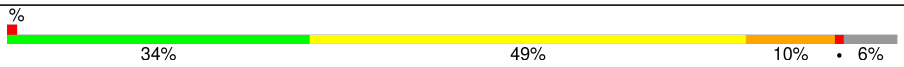
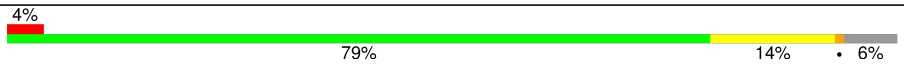
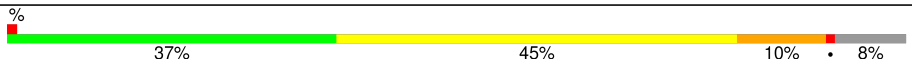
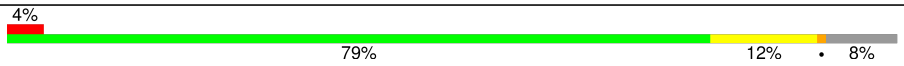
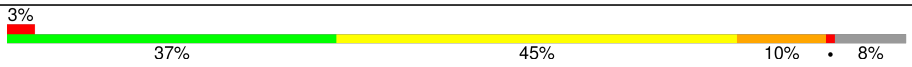
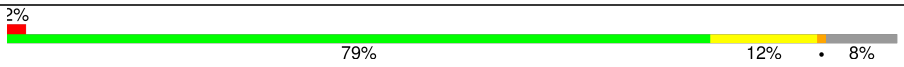
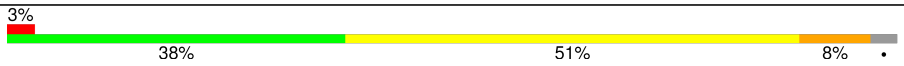
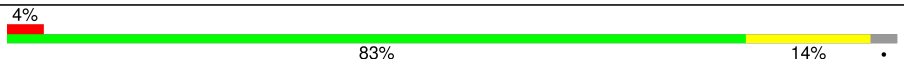
Mol	Chain	Length	Quality of chain
2	Ab	527	
2	BB	527	
2	Bb	527	
3	AD	528	
3	Ad	528	
3	BD	528	
3	Bd	528	
4	AE	562	
4	Ae	562	
4	BE	562	
4	Be	562	
5	AG	590	
5	Ag	590	
5	BG	590	
5	Bg	590	
6	AH	550	
6	Ah	550	
6	BH	550	
6	Bh	550	
7	AQ	568	
7	Aq	568	
7	BQ	568	
7	Bq	568	
8	AZ	546	
8	Az	546	

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Mol	Chain	Length	Quality of chain
8	BZ	546	2% 39% 50% 8%
8	Bz	546	4% 83% 14%

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	AG	1002	-	-	X	-
10	BEF	BG	4002	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 128780 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	AA	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	Aa	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	BA	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			
1	Ba	537	Total	C	N	O	S	0	0	0
			4060	2539	710	791	20			

- Molecule 2 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	Ab	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	BB	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			
2	Bb	517	Total	C	N	O	S	0	0	0
			3927	2455	679	779	14			

- Molecule 3 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	Ad	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	BD	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			
3	Bd	515	Total	C	N	O	S	0	0	0
			3938	2459	694	768	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AD	345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
Ad	1345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
BD	3345	ASP	GLY	ENGINEERED MUTATION	UNP P39078
Bd	4345	ASP	GLY	ENGINEERED MUTATION	UNP P39078

- Molecule 4 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT EPSILON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	Ae	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	BE	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			
4	Be	528	Total	C	N	O	S	0	0	0
			4068	2550	699	798	21			

- Molecule 5 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AG	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	Ag	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	BG	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			
5	Bg	509	Total	C	N	O	S	0	0	0
			3914	2454	686	748	26			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	901	GLY	-	INSERTION	UNP P39077
AG	902	SER	-	INSERTION	UNP P39077
AG	903	GLY	-	INSERTION	UNP P39077
AG	904	SER	-	INSERTION	UNP P39077
AG	905	GLY	-	INSERTION	UNP P39077
AG	906	TRP	-	INSERTION	UNP P39077
AG	907	SER	-	INSERTION	UNP P39077
AG	908	HIS	-	INSERTION	UNP P39077
AG	909	PRO	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
AG	910	GLN	-	INSERTION	UNP P39077
AG	911	PHE	-	INSERTION	UNP P39077
AG	912	GLU	-	INSERTION	UNP P39077
AG	913	LYS	-	INSERTION	UNP P39077
AG	914	GLY	-	INSERTION	UNP P39077
AG	915	SER	-	INSERTION	UNP P39077
AG	916	GLY	-	INSERTION	UNP P39077
AG	917	LYS	-	INSERTION	UNP P39077
AG	918	ARG	-	INSERTION	UNP P39077
AG	919	ARG	-	INSERTION	UNP P39077
AG	920	TRP	-	INSERTION	UNP P39077
AG	921	LYS	-	INSERTION	UNP P39077
AG	922	LYS	-	INSERTION	UNP P39077
AG	923	ASN	-	INSERTION	UNP P39077
AG	924	PHE	-	INSERTION	UNP P39077
AG	925	ILE	-	INSERTION	UNP P39077
AG	926	ALA	-	INSERTION	UNP P39077
AG	927	VAL	-	INSERTION	UNP P39077
AG	928	SER	-	INSERTION	UNP P39077
AG	929	ALA	-	INSERTION	UNP P39077
AG	930	ALA	-	INSERTION	UNP P39077
AG	931	ASN	-	INSERTION	UNP P39077
AG	932	ARG	-	INSERTION	UNP P39077
AG	933	PHE	-	INSERTION	UNP P39077
AG	934	LYS	-	INSERTION	UNP P39077
AG	935	LYS	-	INSERTION	UNP P39077
AG	936	ILE	-	INSERTION	UNP P39077
AG	937	SER	-	INSERTION	UNP P39077
AG	938	SER	-	INSERTION	UNP P39077
AG	939	SER	-	INSERTION	UNP P39077
AG	940	GLY	-	INSERTION	UNP P39077
AG	941	ALA	-	INSERTION	UNP P39077
AG	942	LEU	-	INSERTION	UNP P39077
AG	943	GLY	-	INSERTION	UNP P39077
AG	944	SER	-	INSERTION	UNP P39077
AG	945	GLY	-	INSERTION	UNP P39077
AG	946	HIS	-	INSERTION	UNP P39077
AG	947	HIS	-	INSERTION	UNP P39077
AG	948	HIS	-	INSERTION	UNP P39077
AG	949	HIS	-	INSERTION	UNP P39077
AG	950	HIS	-	INSERTION	UNP P39077
AG	951	HIS	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
AG	952	HIS	-	INSERTION	UNP P39077
AG	953	HIS	-	INSERTION	UNP P39077
AG	954	GLY	-	INSERTION	UNP P39077
AG	955	SER	-	INSERTION	UNP P39077
AG	956	GLY	-	INSERTION	UNP P39077
Ag	1901	GLY	-	INSERTION	UNP P39077
Ag	1902	SER	-	INSERTION	UNP P39077
Ag	1903	GLY	-	INSERTION	UNP P39077
Ag	1904	SER	-	INSERTION	UNP P39077
Ag	1905	GLY	-	INSERTION	UNP P39077
Ag	1906	TRP	-	INSERTION	UNP P39077
Ag	1907	SER	-	INSERTION	UNP P39077
Ag	1908	HIS	-	INSERTION	UNP P39077
Ag	1909	PRO	-	INSERTION	UNP P39077
Ag	1910	GLN	-	INSERTION	UNP P39077
Ag	1911	PHE	-	INSERTION	UNP P39077
Ag	1912	GLU	-	INSERTION	UNP P39077
Ag	1913	LYS	-	INSERTION	UNP P39077
Ag	1914	GLY	-	INSERTION	UNP P39077
Ag	1915	SER	-	INSERTION	UNP P39077
Ag	1916	GLY	-	INSERTION	UNP P39077
Ag	1917	LYS	-	INSERTION	UNP P39077
Ag	1918	ARG	-	INSERTION	UNP P39077
Ag	1919	ARG	-	INSERTION	UNP P39077
Ag	1920	TRP	-	INSERTION	UNP P39077
Ag	1921	LYS	-	INSERTION	UNP P39077
Ag	1922	LYS	-	INSERTION	UNP P39077
Ag	1923	ASN	-	INSERTION	UNP P39077
Ag	1924	PHE	-	INSERTION	UNP P39077
Ag	1925	ILE	-	INSERTION	UNP P39077
Ag	1926	ALA	-	INSERTION	UNP P39077
Ag	1927	VAL	-	INSERTION	UNP P39077
Ag	1928	SER	-	INSERTION	UNP P39077
Ag	1929	ALA	-	INSERTION	UNP P39077
Ag	1930	ALA	-	INSERTION	UNP P39077
Ag	1931	ASN	-	INSERTION	UNP P39077
Ag	1932	ARG	-	INSERTION	UNP P39077
Ag	1933	PHE	-	INSERTION	UNP P39077
Ag	1934	LYS	-	INSERTION	UNP P39077
Ag	1935	LYS	-	INSERTION	UNP P39077
Ag	1936	ILE	-	INSERTION	UNP P39077
Ag	1937	SER	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Ag	1938	SER	-	INSERTION	UNP P39077
Ag	1939	SER	-	INSERTION	UNP P39077
Ag	1940	GLY	-	INSERTION	UNP P39077
Ag	1941	ALA	-	INSERTION	UNP P39077
Ag	1942	LEU	-	INSERTION	UNP P39077
Ag	1943	GLY	-	INSERTION	UNP P39077
Ag	1944	SER	-	INSERTION	UNP P39077
Ag	1945	GLY	-	INSERTION	UNP P39077
Ag	1946	HIS	-	INSERTION	UNP P39077
Ag	1947	HIS	-	INSERTION	UNP P39077
Ag	1948	HIS	-	INSERTION	UNP P39077
Ag	1949	HIS	-	INSERTION	UNP P39077
Ag	1950	HIS	-	INSERTION	UNP P39077
Ag	1951	HIS	-	INSERTION	UNP P39077
Ag	1952	HIS	-	INSERTION	UNP P39077
Ag	1953	HIS	-	INSERTION	UNP P39077
Ag	1954	GLY	-	INSERTION	UNP P39077
Ag	1955	SER	-	INSERTION	UNP P39077
Ag	1956	GLY	-	INSERTION	UNP P39077
BG	3901	GLY	-	INSERTION	UNP P39077
BG	3902	SER	-	INSERTION	UNP P39077
BG	3903	GLY	-	INSERTION	UNP P39077
BG	3904	SER	-	INSERTION	UNP P39077
BG	3905	GLY	-	INSERTION	UNP P39077
BG	3906	TRP	-	INSERTION	UNP P39077
BG	3907	SER	-	INSERTION	UNP P39077
BG	3908	HIS	-	INSERTION	UNP P39077
BG	3909	PRO	-	INSERTION	UNP P39077
BG	3910	GLN	-	INSERTION	UNP P39077
BG	3911	PHE	-	INSERTION	UNP P39077
BG	3912	GLU	-	INSERTION	UNP P39077
BG	3913	LYS	-	INSERTION	UNP P39077
BG	3914	GLY	-	INSERTION	UNP P39077
BG	3915	SER	-	INSERTION	UNP P39077
BG	3916	GLY	-	INSERTION	UNP P39077
BG	3917	LYS	-	INSERTION	UNP P39077
BG	3918	ARG	-	INSERTION	UNP P39077
BG	3919	ARG	-	INSERTION	UNP P39077
BG	3920	TRP	-	INSERTION	UNP P39077
BG	3921	LYS	-	INSERTION	UNP P39077
BG	3922	LYS	-	INSERTION	UNP P39077
BG	3923	ASN	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
BG	3924	PHE	-	INSERTION	UNP P39077
BG	3925	ILE	-	INSERTION	UNP P39077
BG	3926	ALA	-	INSERTION	UNP P39077
BG	3927	VAL	-	INSERTION	UNP P39077
BG	3928	SER	-	INSERTION	UNP P39077
BG	3929	ALA	-	INSERTION	UNP P39077
BG	3930	ALA	-	INSERTION	UNP P39077
BG	3931	ASN	-	INSERTION	UNP P39077
BG	3932	ARG	-	INSERTION	UNP P39077
BG	3933	PHE	-	INSERTION	UNP P39077
BG	3934	LYS	-	INSERTION	UNP P39077
BG	3935	LYS	-	INSERTION	UNP P39077
BG	3936	ILE	-	INSERTION	UNP P39077
BG	3937	SER	-	INSERTION	UNP P39077
BG	3938	SER	-	INSERTION	UNP P39077
BG	3939	SER	-	INSERTION	UNP P39077
BG	3940	GLY	-	INSERTION	UNP P39077
BG	3941	ALA	-	INSERTION	UNP P39077
BG	3942	LEU	-	INSERTION	UNP P39077
BG	3943	GLY	-	INSERTION	UNP P39077
BG	3944	SER	-	INSERTION	UNP P39077
BG	3945	GLY	-	INSERTION	UNP P39077
BG	3946	HIS	-	INSERTION	UNP P39077
BG	3947	HIS	-	INSERTION	UNP P39077
BG	3948	HIS	-	INSERTION	UNP P39077
BG	3949	HIS	-	INSERTION	UNP P39077
BG	3950	HIS	-	INSERTION	UNP P39077
BG	3951	HIS	-	INSERTION	UNP P39077
BG	3952	HIS	-	INSERTION	UNP P39077
BG	3953	HIS	-	INSERTION	UNP P39077
BG	3954	GLY	-	INSERTION	UNP P39077
BG	3955	SER	-	INSERTION	UNP P39077
BG	3956	GLY	-	INSERTION	UNP P39077
Bg	4901	GLY	-	INSERTION	UNP P39077
Bg	4902	SER	-	INSERTION	UNP P39077
Bg	4903	GLY	-	INSERTION	UNP P39077
Bg	4904	SER	-	INSERTION	UNP P39077
Bg	4905	GLY	-	INSERTION	UNP P39077
Bg	4906	TRP	-	INSERTION	UNP P39077
Bg	4907	SER	-	INSERTION	UNP P39077
Bg	4908	HIS	-	INSERTION	UNP P39077
Bg	4909	PRO	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	4910	GLN	-	INSERTION	UNP P39077
Bg	4911	PHE	-	INSERTION	UNP P39077
Bg	4912	GLU	-	INSERTION	UNP P39077
Bg	4913	LYS	-	INSERTION	UNP P39077
Bg	4914	GLY	-	INSERTION	UNP P39077
Bg	4915	SER	-	INSERTION	UNP P39077
Bg	4916	GLY	-	INSERTION	UNP P39077
Bg	4917	LYS	-	INSERTION	UNP P39077
Bg	4918	ARG	-	INSERTION	UNP P39077
Bg	4919	ARG	-	INSERTION	UNP P39077
Bg	4920	TRP	-	INSERTION	UNP P39077
Bg	4921	LYS	-	INSERTION	UNP P39077
Bg	4922	LYS	-	INSERTION	UNP P39077
Bg	4923	ASN	-	INSERTION	UNP P39077
Bg	4924	PHE	-	INSERTION	UNP P39077
Bg	4925	ILE	-	INSERTION	UNP P39077
Bg	4926	ALA	-	INSERTION	UNP P39077
Bg	4927	VAL	-	INSERTION	UNP P39077
Bg	4928	SER	-	INSERTION	UNP P39077
Bg	4929	ALA	-	INSERTION	UNP P39077
Bg	4930	ALA	-	INSERTION	UNP P39077
Bg	4931	ASN	-	INSERTION	UNP P39077
Bg	4932	ARG	-	INSERTION	UNP P39077
Bg	4933	PHE	-	INSERTION	UNP P39077
Bg	4934	LYS	-	INSERTION	UNP P39077
Bg	4935	LYS	-	INSERTION	UNP P39077
Bg	4936	ILE	-	INSERTION	UNP P39077
Bg	4937	SER	-	INSERTION	UNP P39077
Bg	4938	SER	-	INSERTION	UNP P39077
Bg	4939	SER	-	INSERTION	UNP P39077
Bg	4940	GLY	-	INSERTION	UNP P39077
Bg	4941	ALA	-	INSERTION	UNP P39077
Bg	4942	LEU	-	INSERTION	UNP P39077
Bg	4943	GLY	-	INSERTION	UNP P39077
Bg	4944	SER	-	INSERTION	UNP P39077
Bg	4945	GLY	-	INSERTION	UNP P39077
Bg	4946	HIS	-	INSERTION	UNP P39077
Bg	4947	HIS	-	INSERTION	UNP P39077
Bg	4948	HIS	-	INSERTION	UNP P39077
Bg	4949	HIS	-	INSERTION	UNP P39077
Bg	4950	HIS	-	INSERTION	UNP P39077
Bg	4951	HIS	-	INSERTION	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	4952	HIS	-	INSERTION	UNP P39077
Bg	4953	HIS	-	INSERTION	UNP P39077
Bg	4954	GLY	-	INSERTION	UNP P39077
Bg	4955	SER	-	INSERTION	UNP P39077
Bg	4956	GLY	-	INSERTION	UNP P39077

- Molecule 6 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AH	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	Ah	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	BH	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			
6	Bh	519	Total	C	N	O	S	0	0	0
			3962	2495	678	770	19			

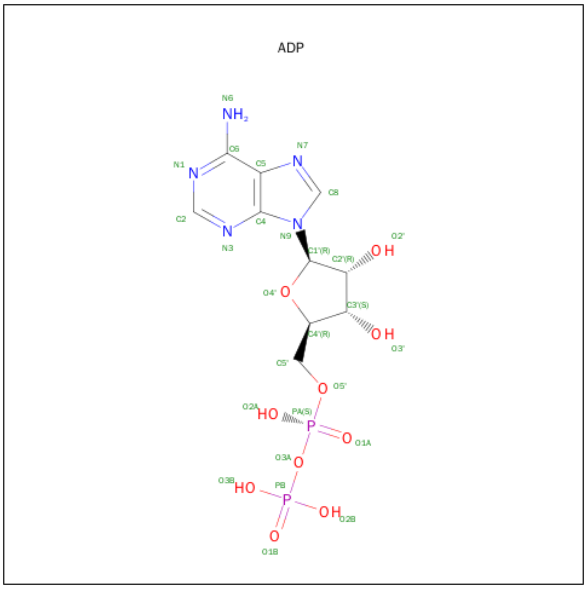
- Molecule 7 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT THETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AQ	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	Aq	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	BQ	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			
7	Bq	523	Total	C	N	O	S	0	0	0
			3981	2509	680	766	26			

- Molecule 8 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ZETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AZ	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	Az	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	BZ	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			
8	Bz	531	Total	C	N	O	S	0	0	0
			4089	2570	708	794	17			

- 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	AA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AE	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AG	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AH	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	AZ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Aa	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ab	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ad	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ae	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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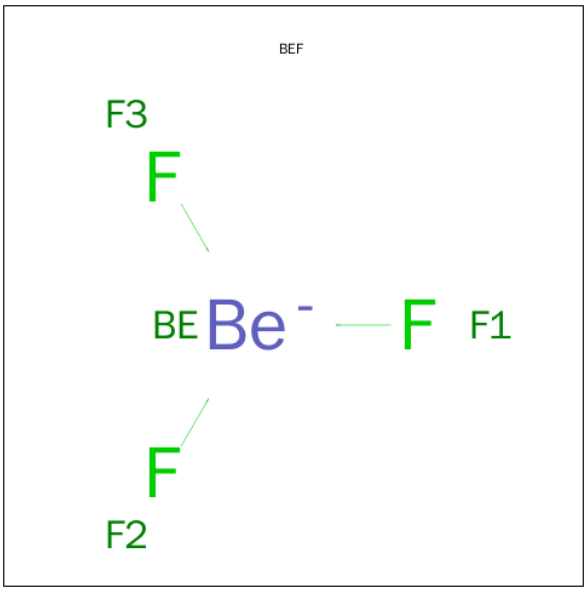
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Ag	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ah	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Aq	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Az	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BA	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BB	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BD	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BE	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BG	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BH	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BQ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	BZ	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Ba	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bb	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bd	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Be	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bg	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bh	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bq	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	Bz	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	AA	1	Total Be F 4 1 3	0	0
10	AB	1	Total Be F 4 1 3	0	0
10	AD	1	Total Be F 4 1 3	0	0
10	AE	1	Total Be F 4 1 3	0	0
10	AG	1	Total Be F 4 1 3	0	0
10	AH	1	Total Be F 4 1 3	0	0
10	AQ	1	Total Be F 4 1 3	0	0
10	AZ	1	Total Be F 4 1 3	0	0
10	Aa	1	Total Be F 4 1 3	0	0
10	Ab	1	Total Be F 4 1 3	0	0
10	Ad	1	Total Be F 4 1 3	0	0
10	Ae	1	Total Be F 4 1 3	0	0
10	Ag	1	Total Be F 4 1 3	0	0
10	Ah	1	Total Be F 4 1 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	Aq	1	Total Be F 4 1 3	0	0
10	Az	1	Total Be F 4 1 3	0	0
10	BA	1	Total Be F 4 1 3	0	0
10	BB	1	Total Be F 4 1 3	0	0
10	BD	1	Total Be F 4 1 3	0	0
10	BE	1	Total Be F 4 1 3	0	0
10	BG	1	Total Be F 4 1 3	0	0
10	BH	1	Total Be F 4 1 3	0	0
10	BQ	1	Total Be F 4 1 3	0	0
10	BZ	1	Total Be F 4 1 3	0	0
10	Ba	1	Total Be F 4 1 3	0	0
10	Bb	1	Total Be F 4 1 3	0	0
10	Bd	1	Total Be F 4 1 3	0	0
10	Be	1	Total Be F 4 1 3	0	0
10	Bg	1	Total Be F 4 1 3	0	0
10	Bh	1	Total Be F 4 1 3	0	0
10	Bq	1	Total Be F 4 1 3	0	0
10	Bz	1	Total Be F 4 1 3	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	Ag	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	Aq	1	Total Mg 1 1	0	0
11	BA	1	Total Mg 1 1	0	0
11	Ah	1	Total Mg 1 1	0	0
11	Bz	1	Total Mg 1 1	0	0
11	AB	1	Total Mg 1 1	0	0
11	BE	1	Total Mg 1 1	0	0
11	Bd	1	Total Mg 1 1	0	0
11	Bh	1	Total Mg 1 1	0	0
11	BB	1	Total Mg 1 1	0	0
11	Ba	1	Total Mg 1 1	0	0
11	AE	1	Total Mg 1 1	0	0
11	Ab	1	Total Mg 1 1	0	0
11	Be	1	Total Mg 1 1	0	0
11	AA	1	Total Mg 1 1	0	0
11	BQ	1	Total Mg 1 1	0	0
11	Bb	1	Total Mg 1 1	0	0
11	AD	1	Total Mg 1 1	0	0
11	Ae	1	Total Mg 1 1	0	0
11	BG	1	Total Mg 1 1	0	0
11	AZ	1	Total Mg 1 1	0	0
11	Aa	1	Total Mg 1 1	0	0

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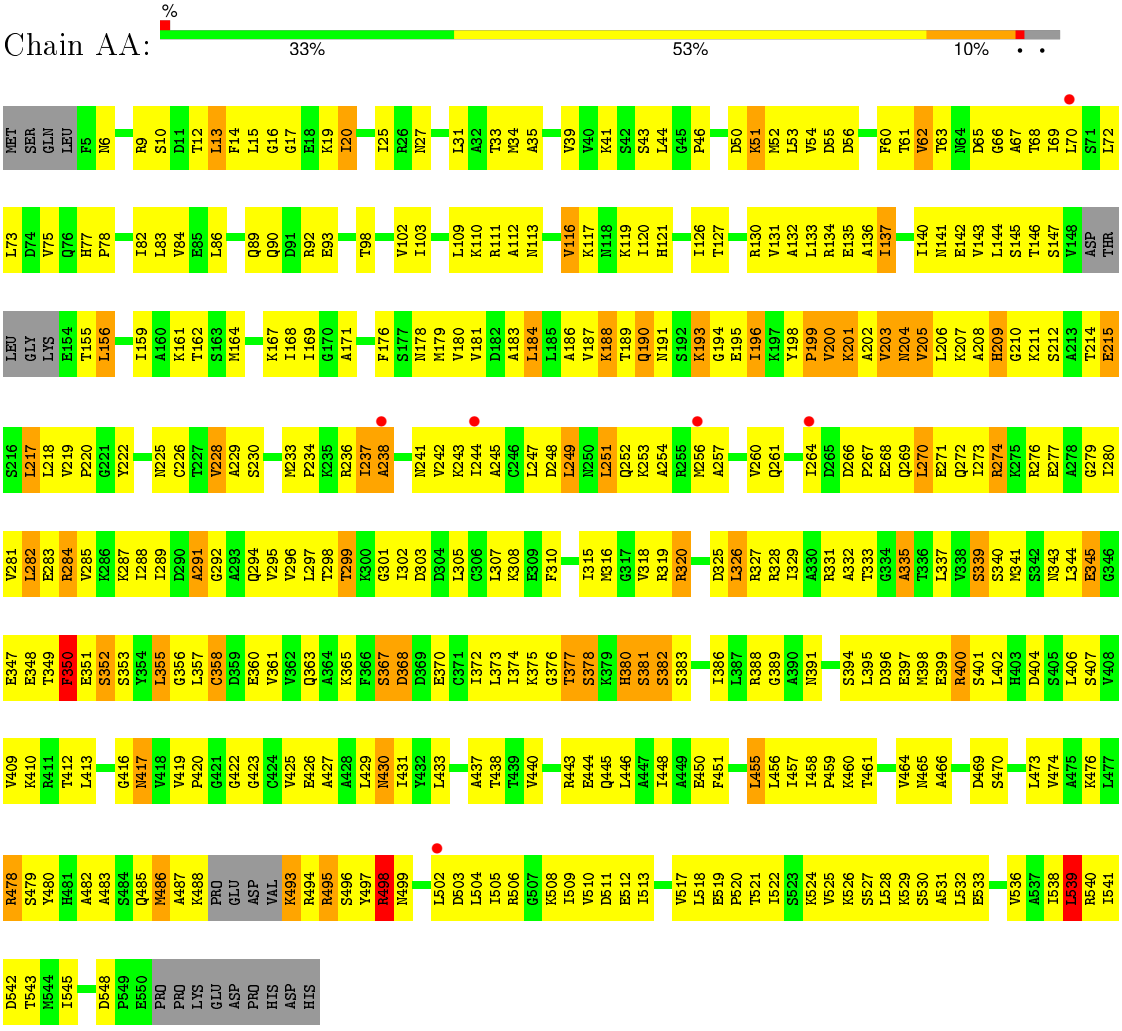
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	Bq	1	Total Mg 1 1	0	0
11	AG	1	Total Mg 1 1	0	0
11	AQ	1	Total Mg 1 1	0	0
11	Ad	1	Total Mg 1 1	0	0
11	AH	1	Total Mg 1 1	0	0
11	BZ	1	Total Mg 1 1	0	0
11	Bg	1	Total Mg 1 1	0	0
11	Az	1	Total Mg 1 1	0	0
11	BD	1	Total Mg 1 1	0	0
11	BH	1	Total Mg 1 1	0	0

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.

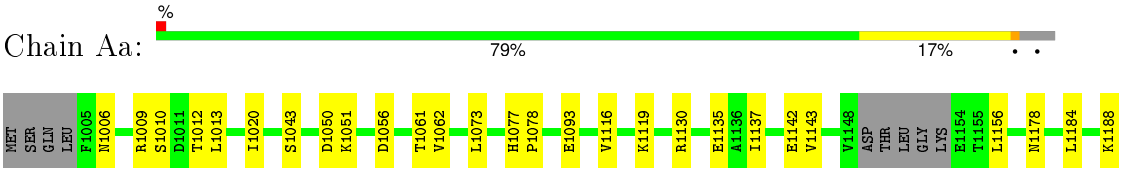
- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA

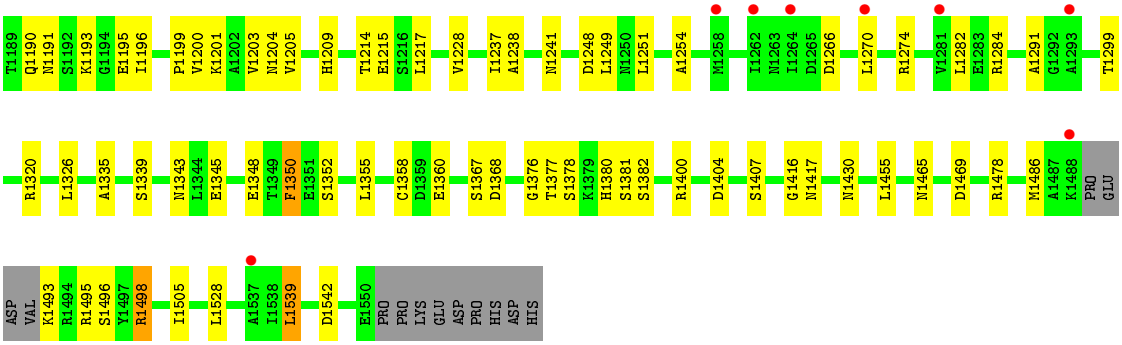
Chain AA:



- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA

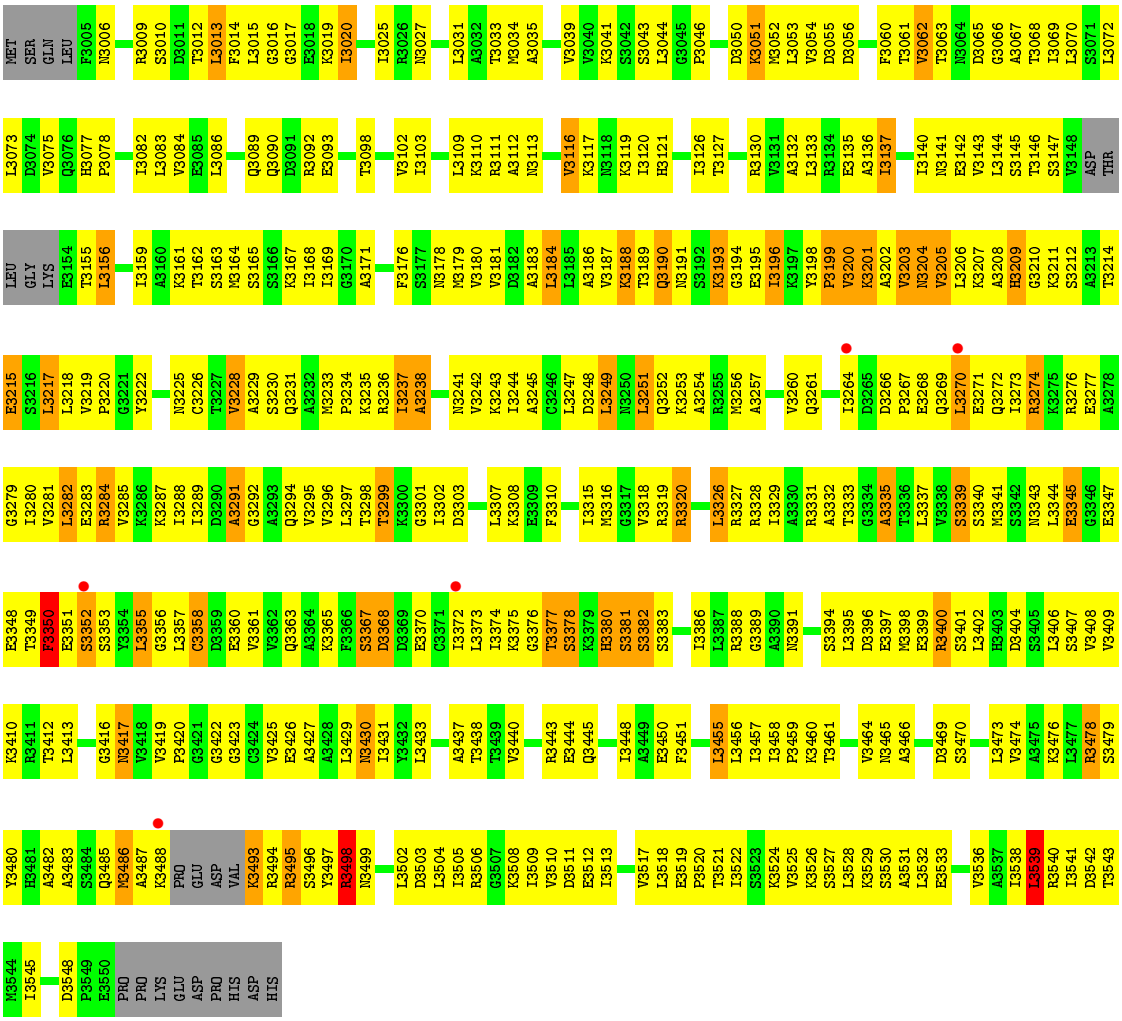
Chain Aa:





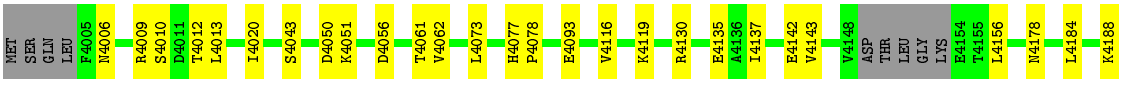
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA

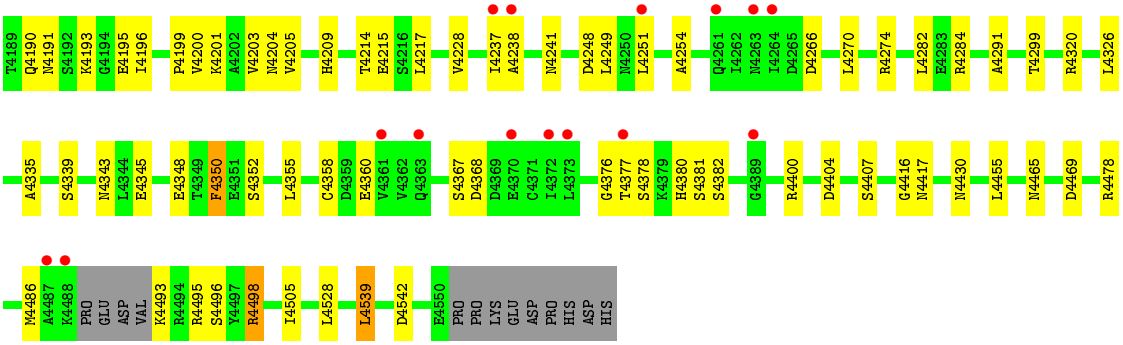
Chain BA:



• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA

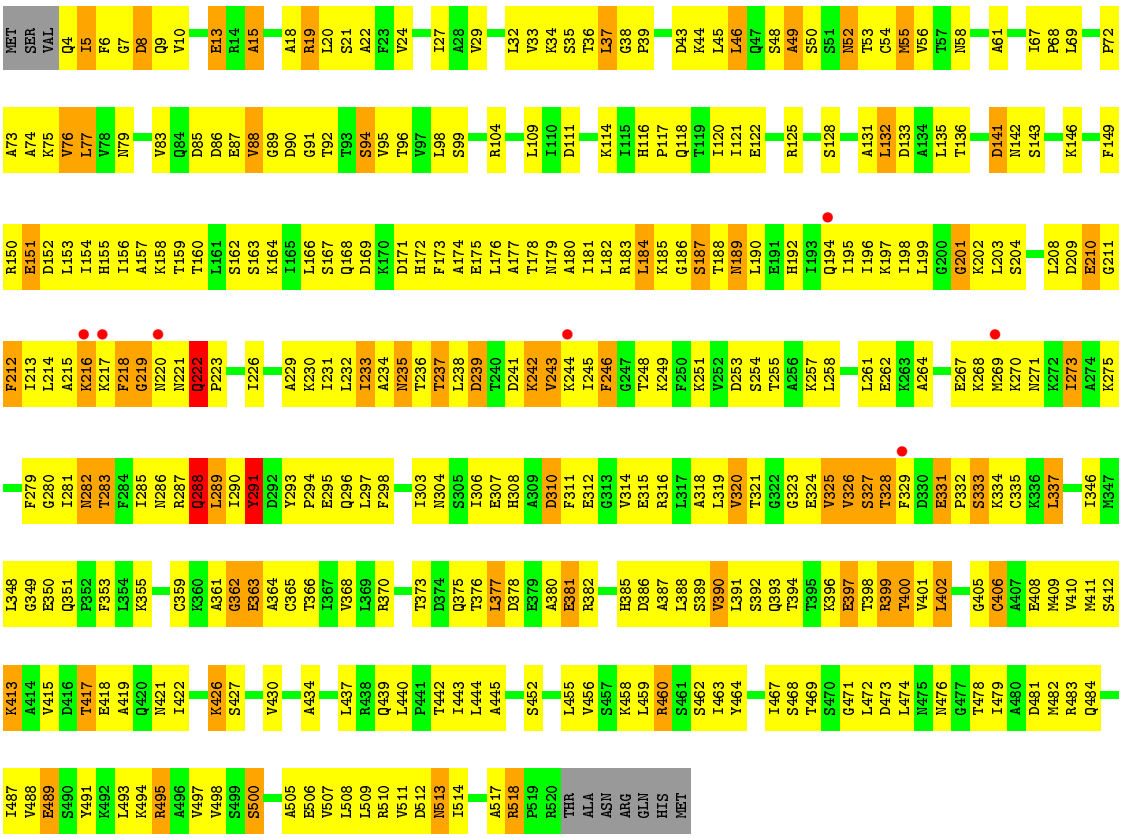
Chain Ba:





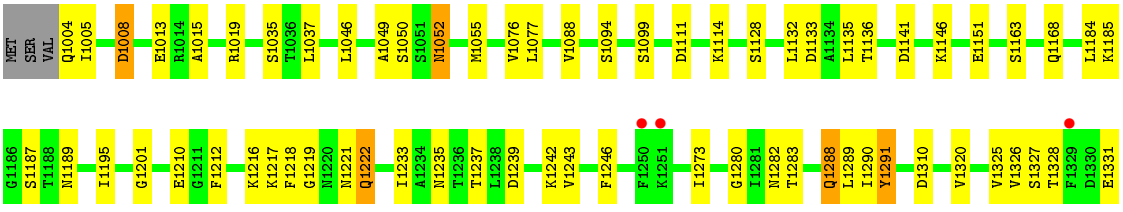
• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain AB:



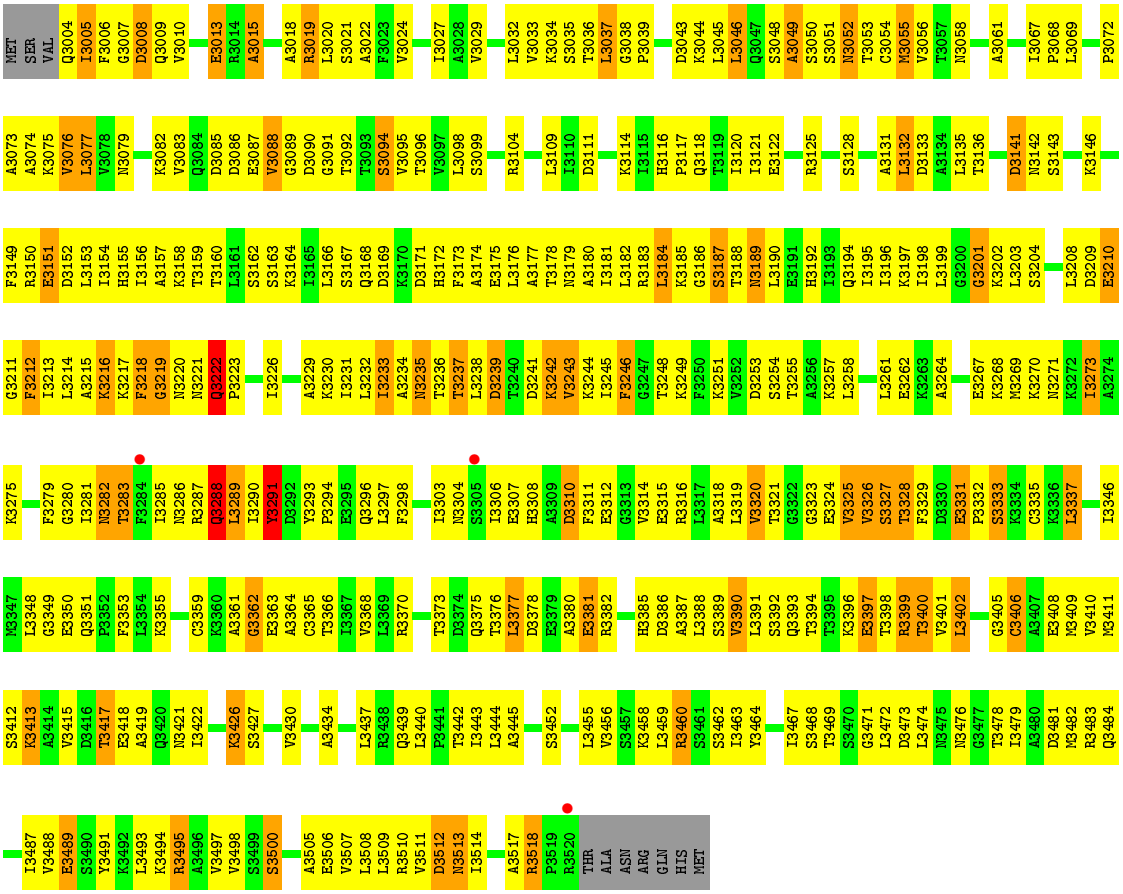
• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain Ab:



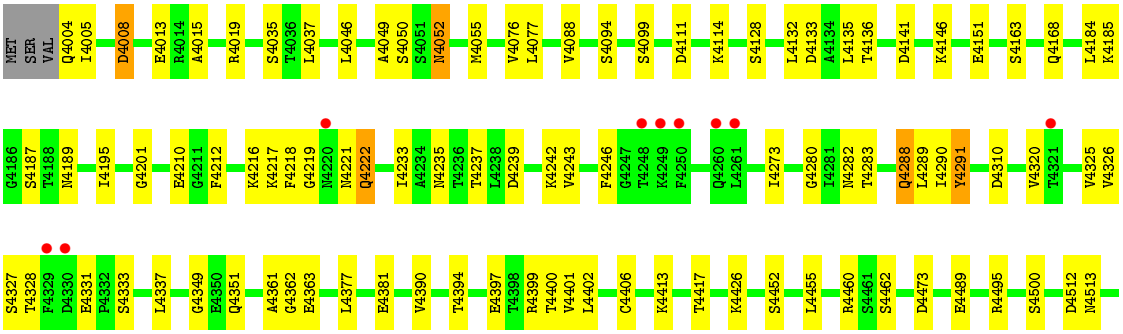
• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain BB:



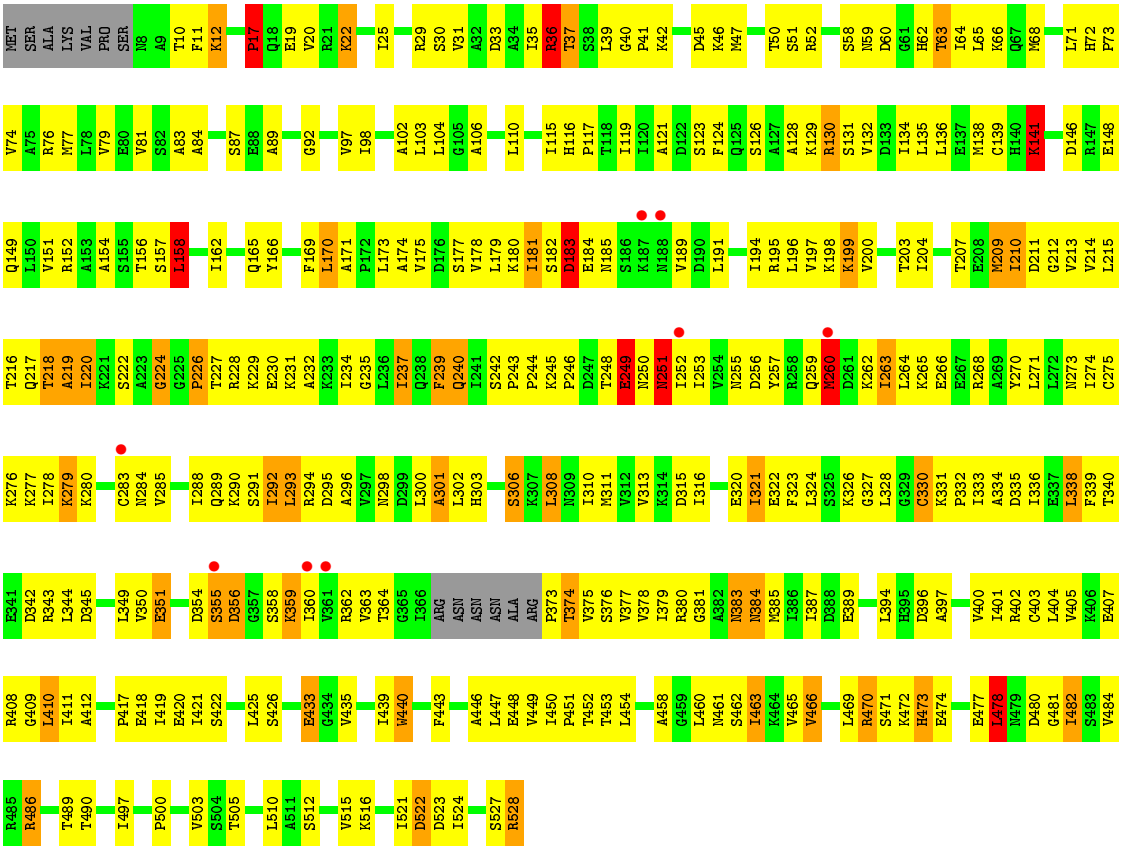
• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

Chain Bb:



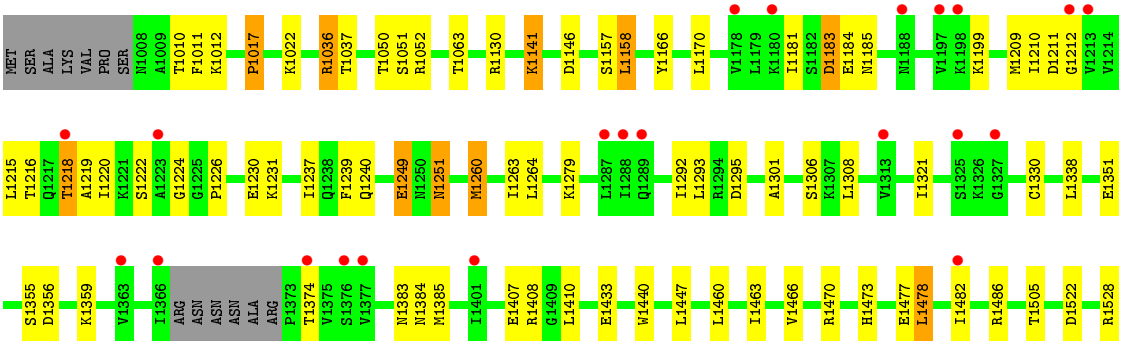
• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

Chain AD:



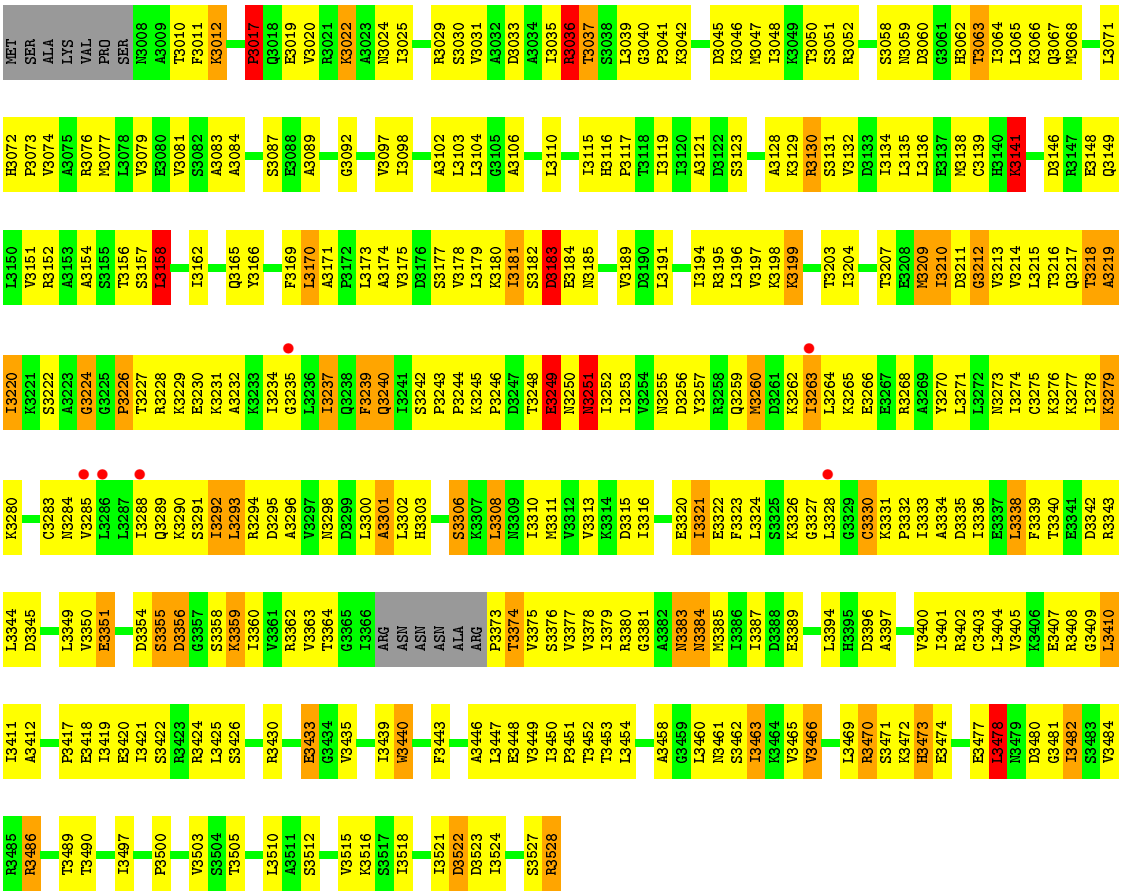
• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

Chain Ad:



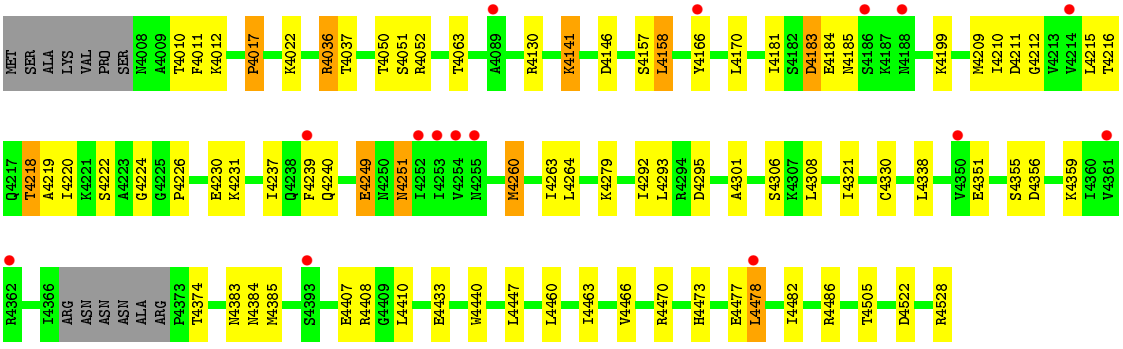
• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

Chain BD:



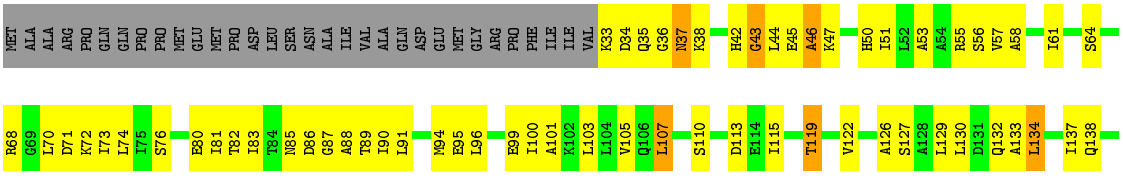
• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

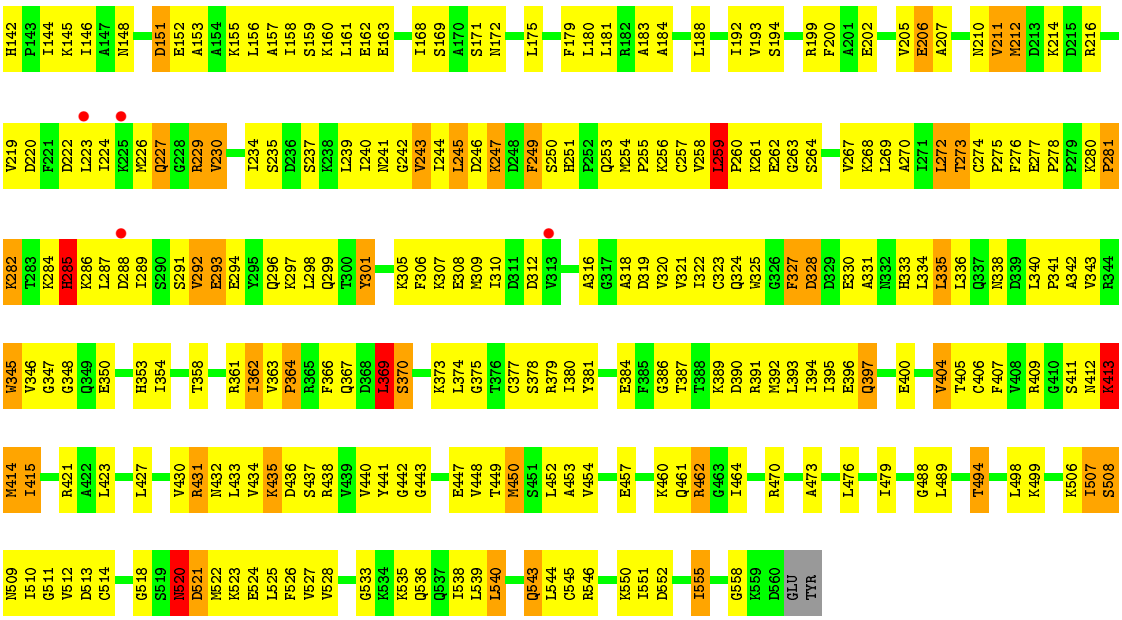
Chain Bd:



• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

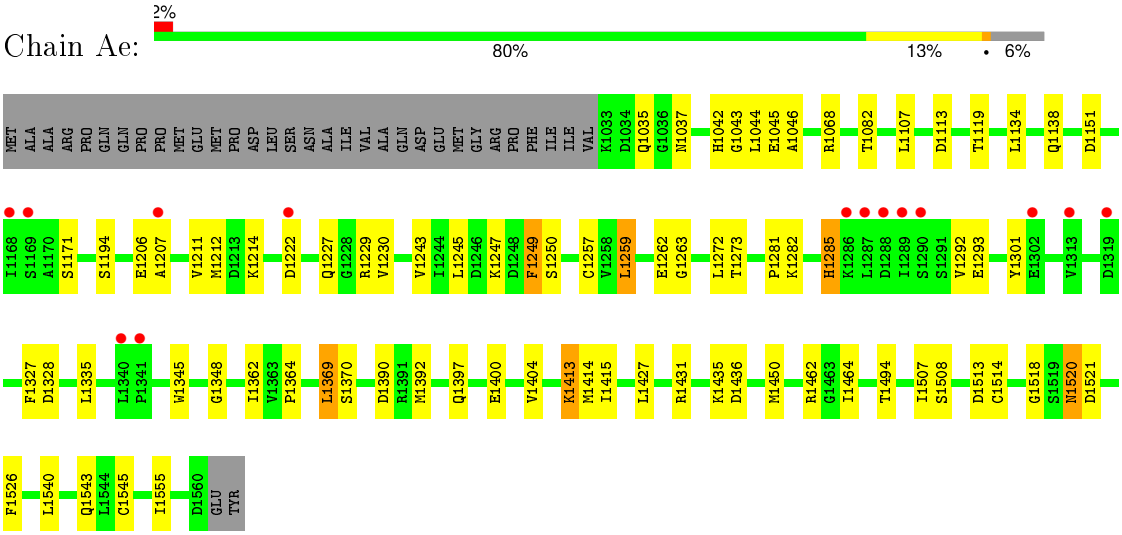
Chain AE:





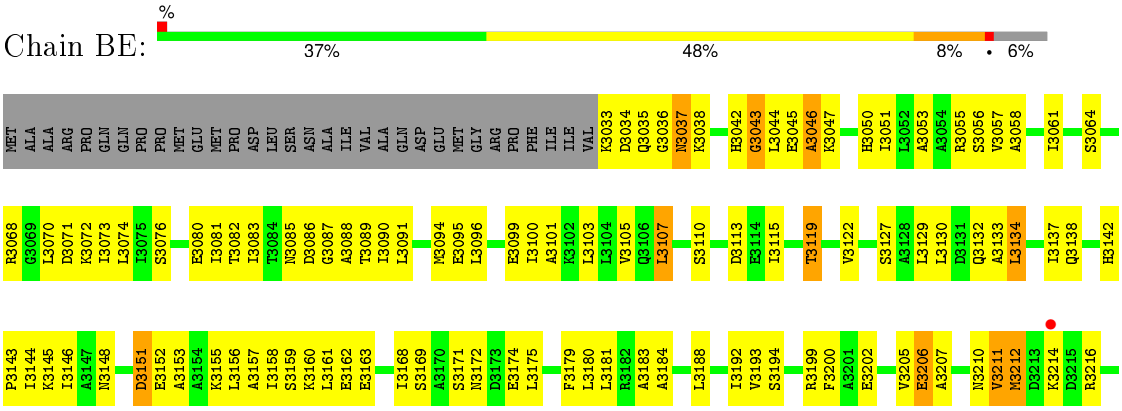
• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

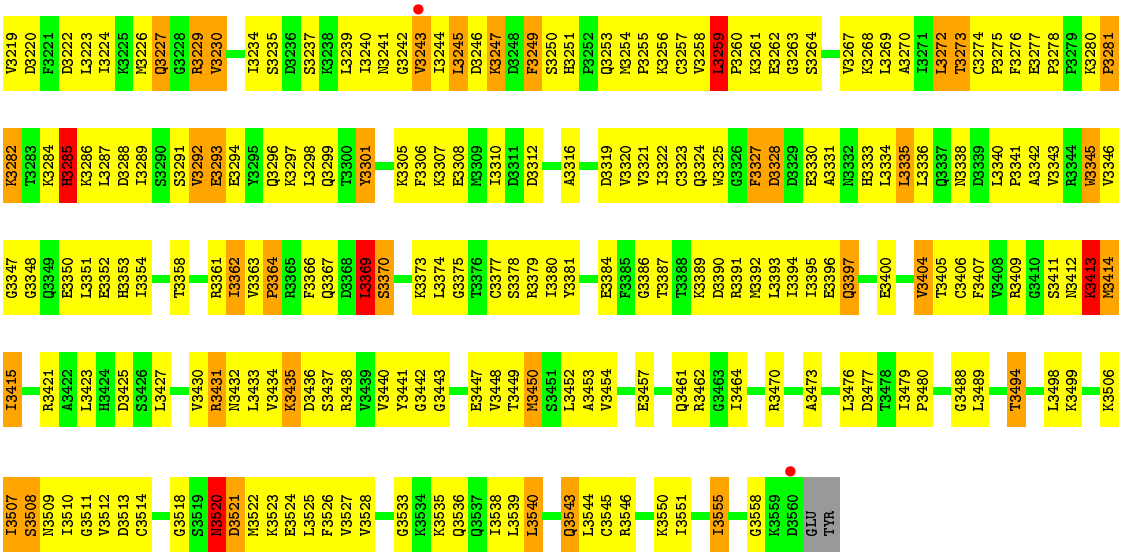
Chain Ae:



• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

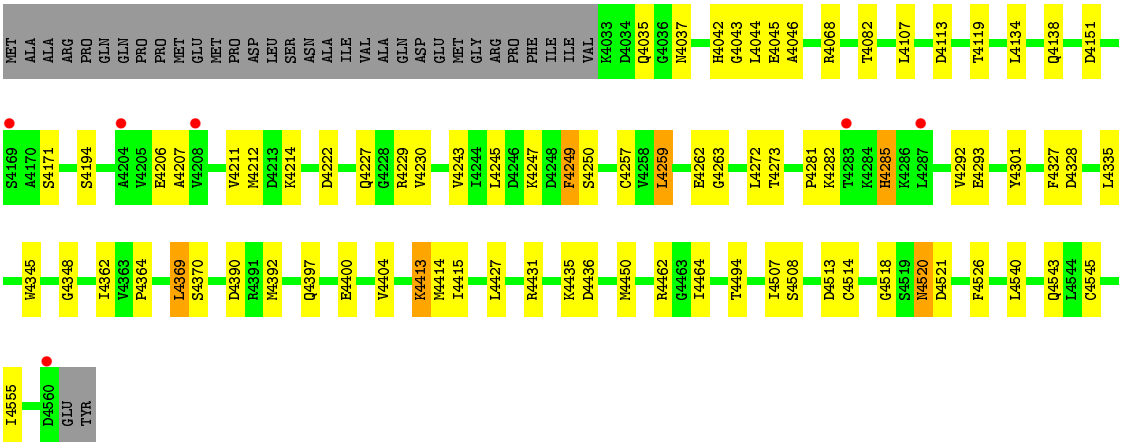
Chain BE:





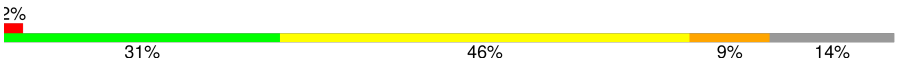
• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

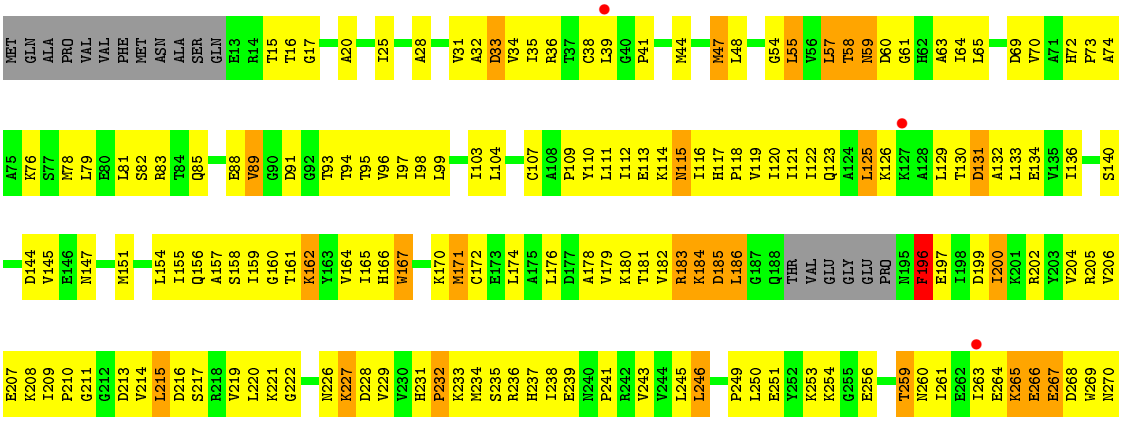
Chain Be:

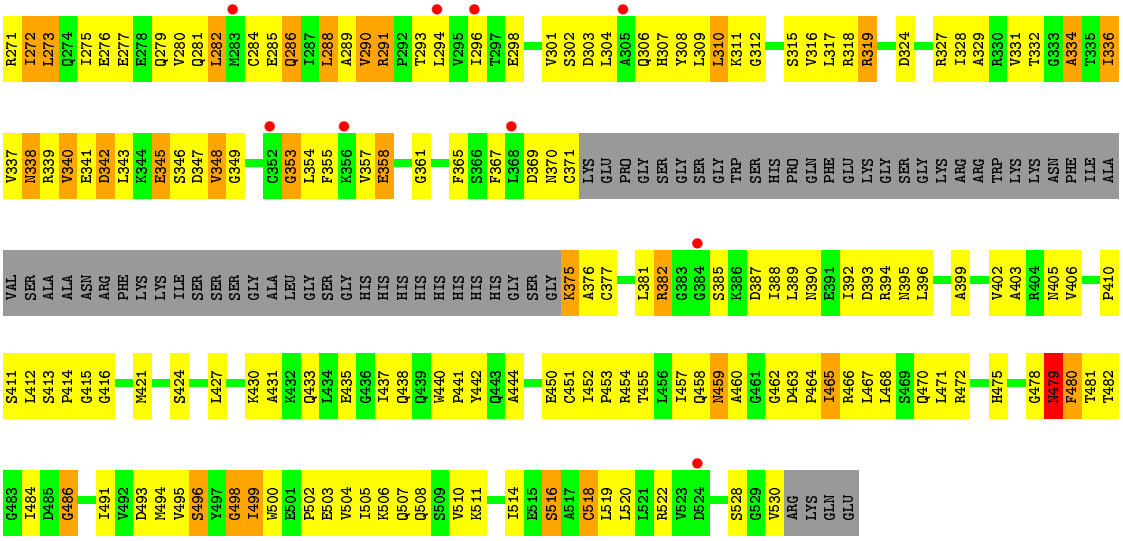


• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

Chain AG:

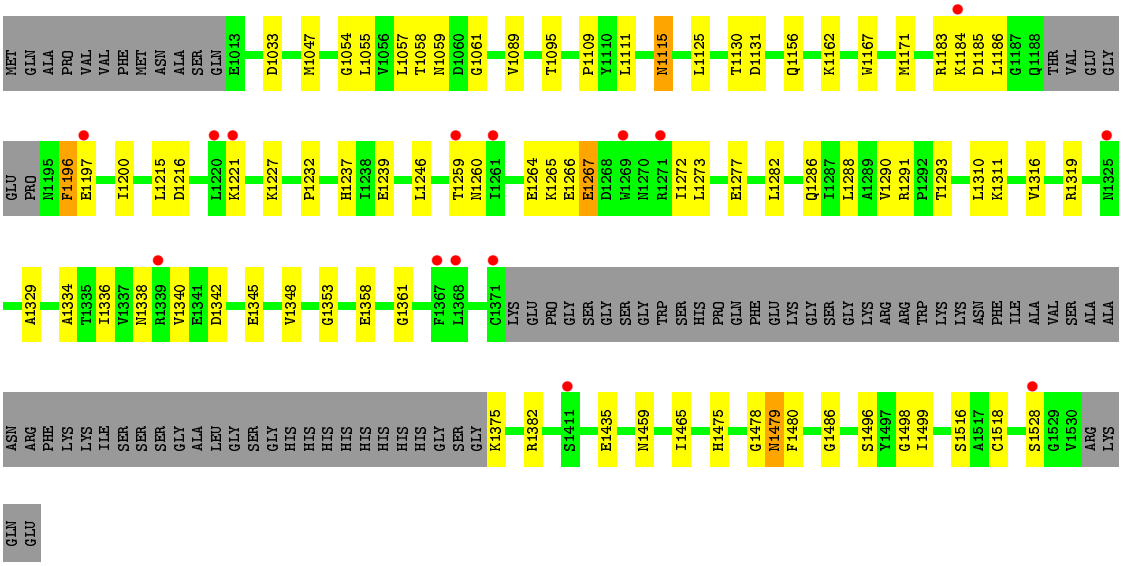






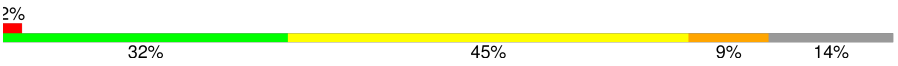
• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

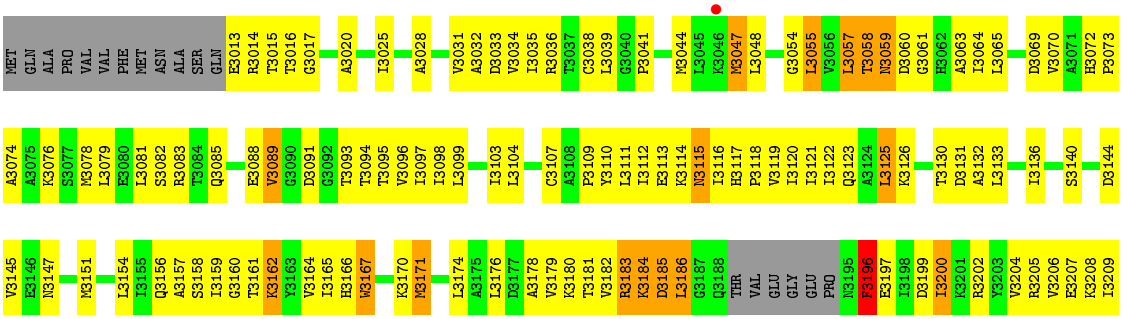
Chain Ag:

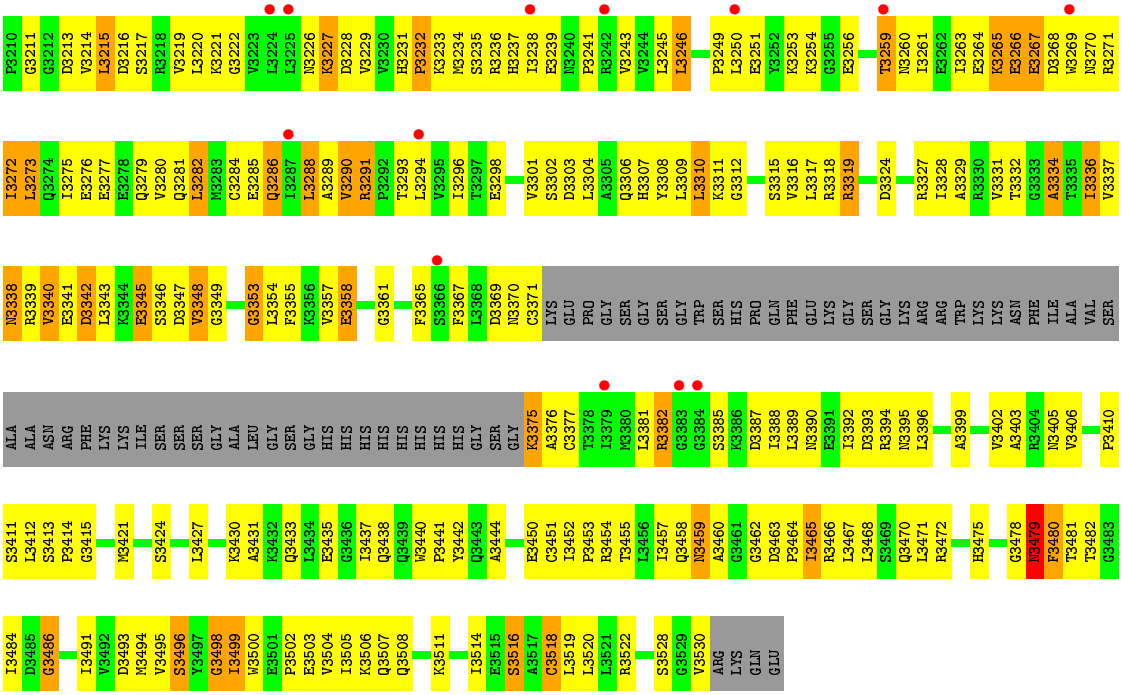


• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

Chain BG:

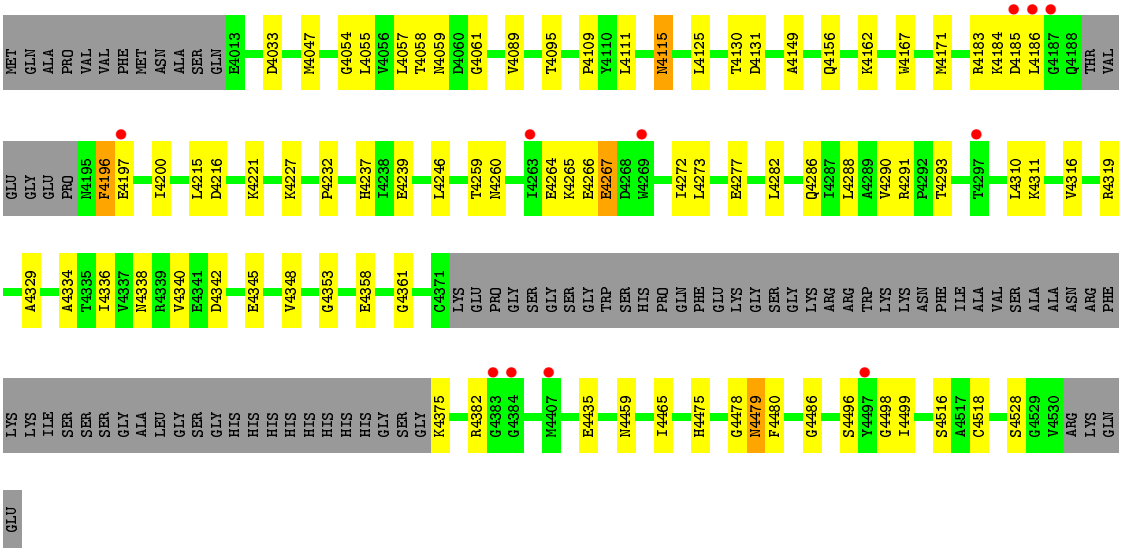






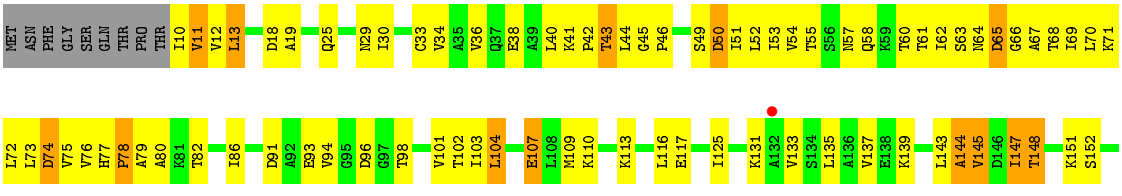
• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

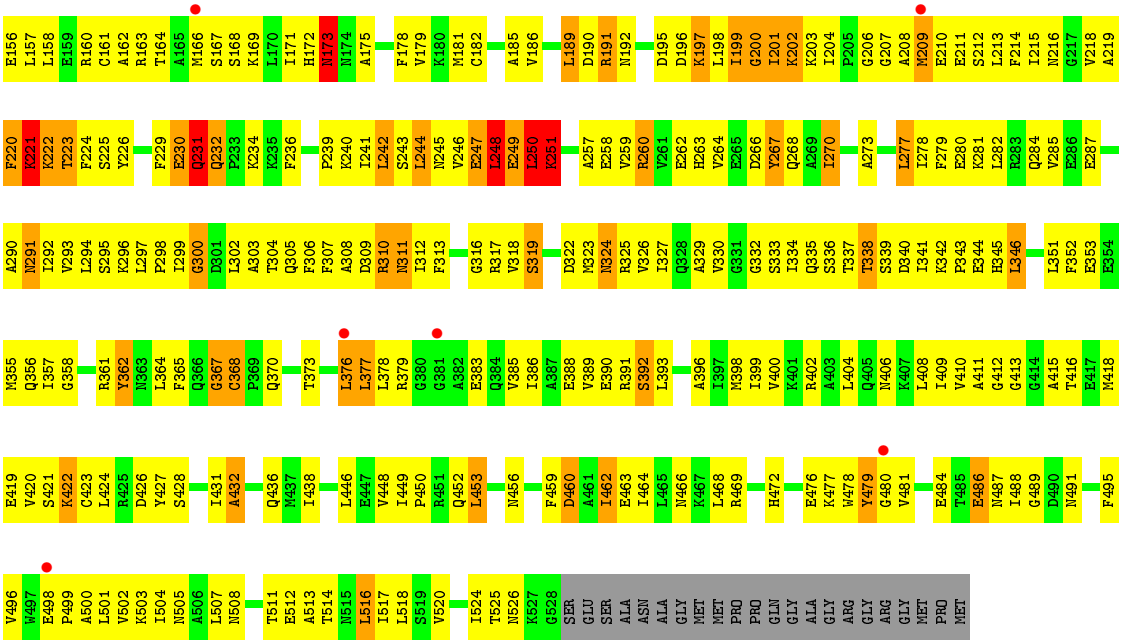
Chain Bg:



• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

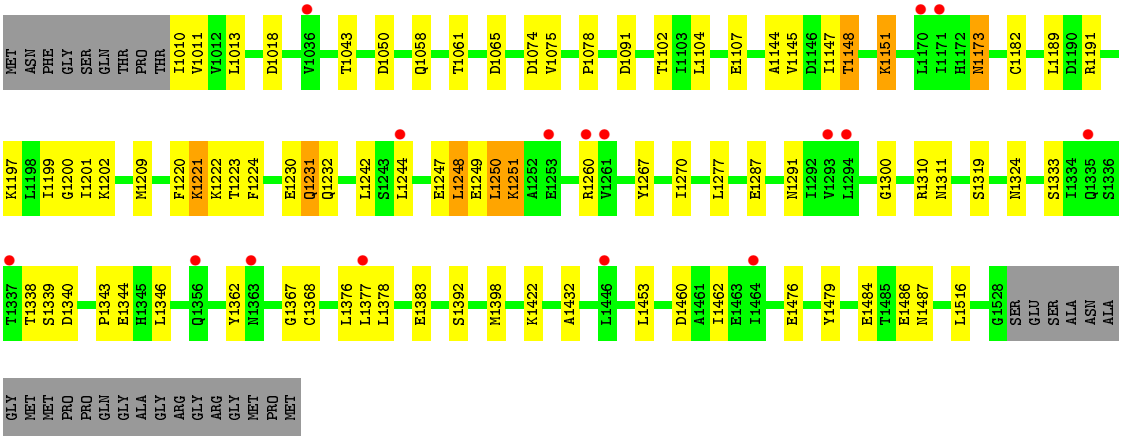
Chain AH:





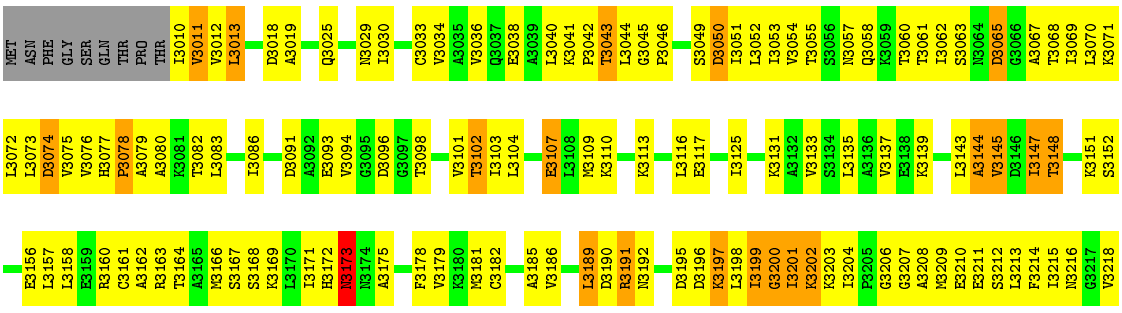
• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

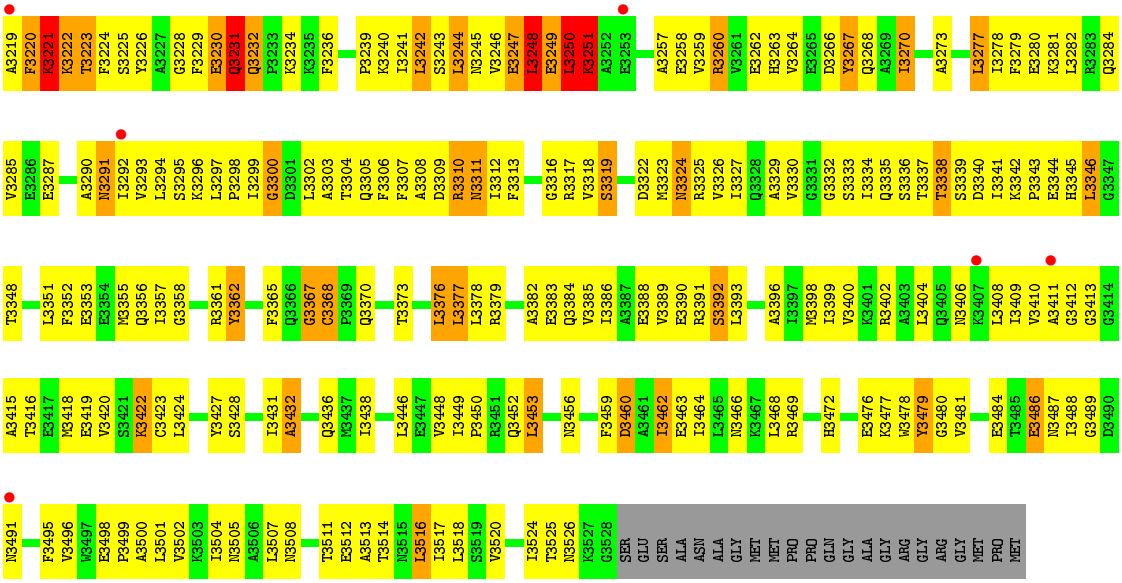
Chain Ah:



• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

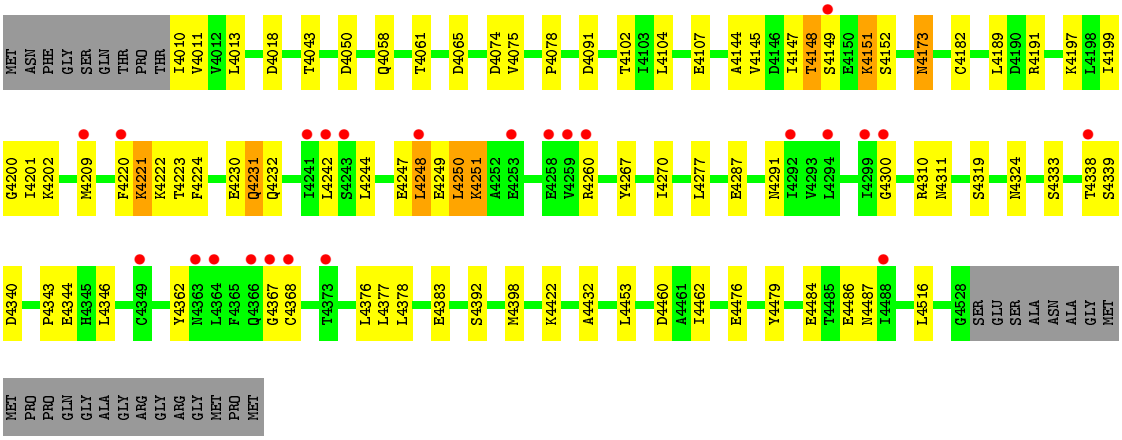
Chain BH:





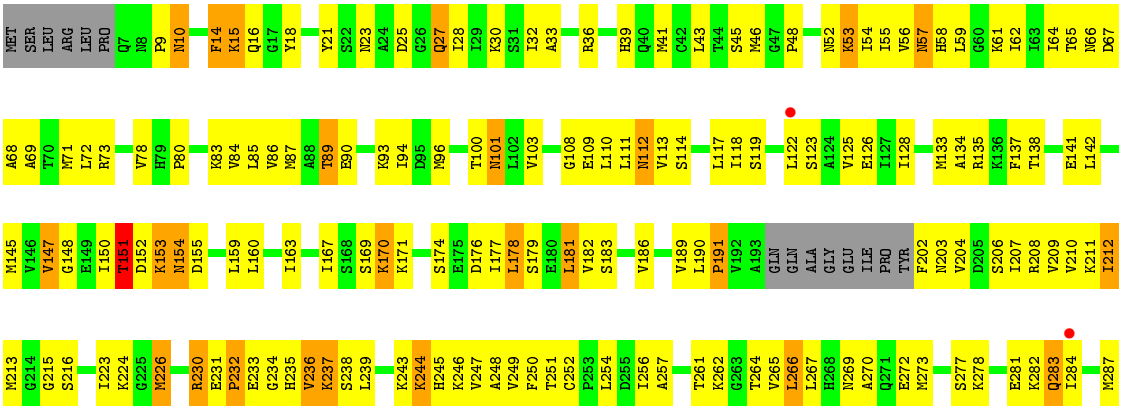
• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

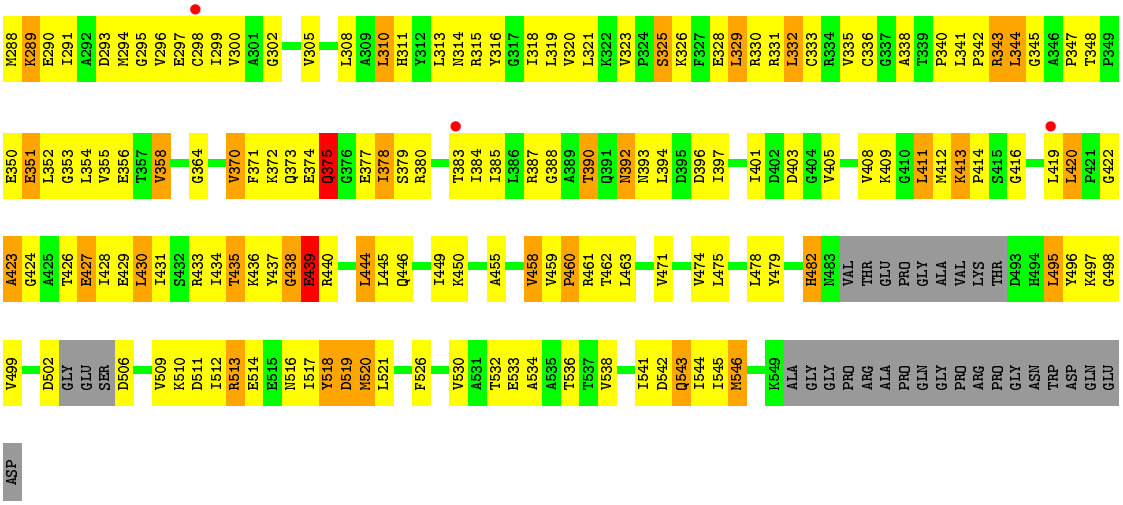
Chain Bh:



• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

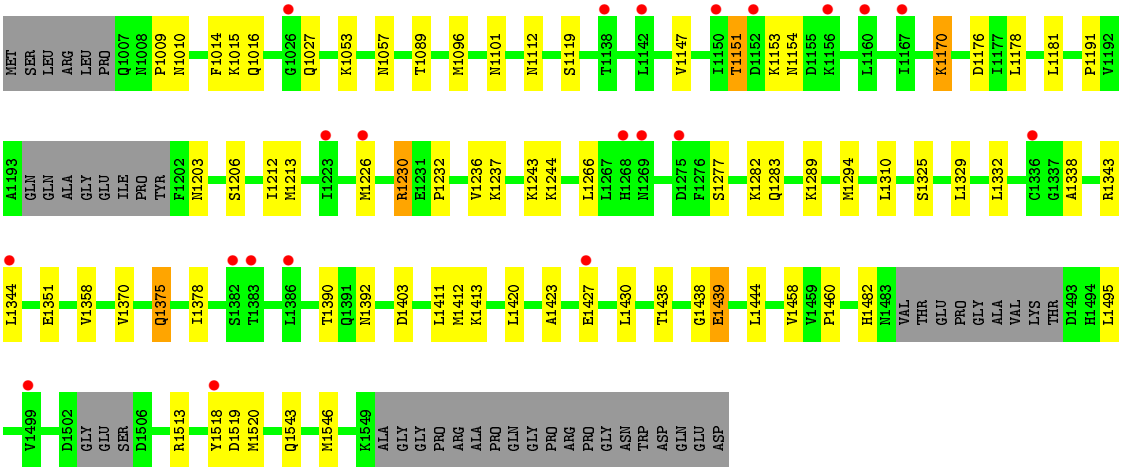
Chain AQ:





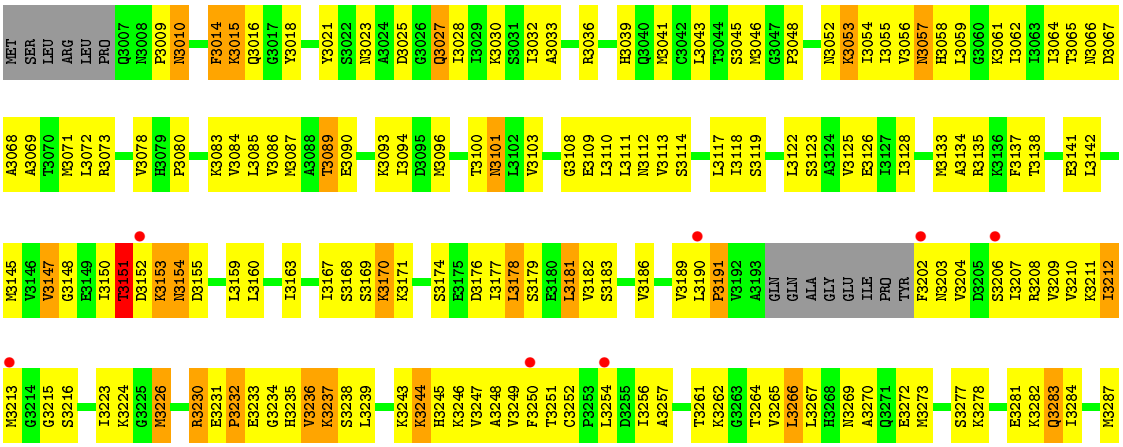
• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

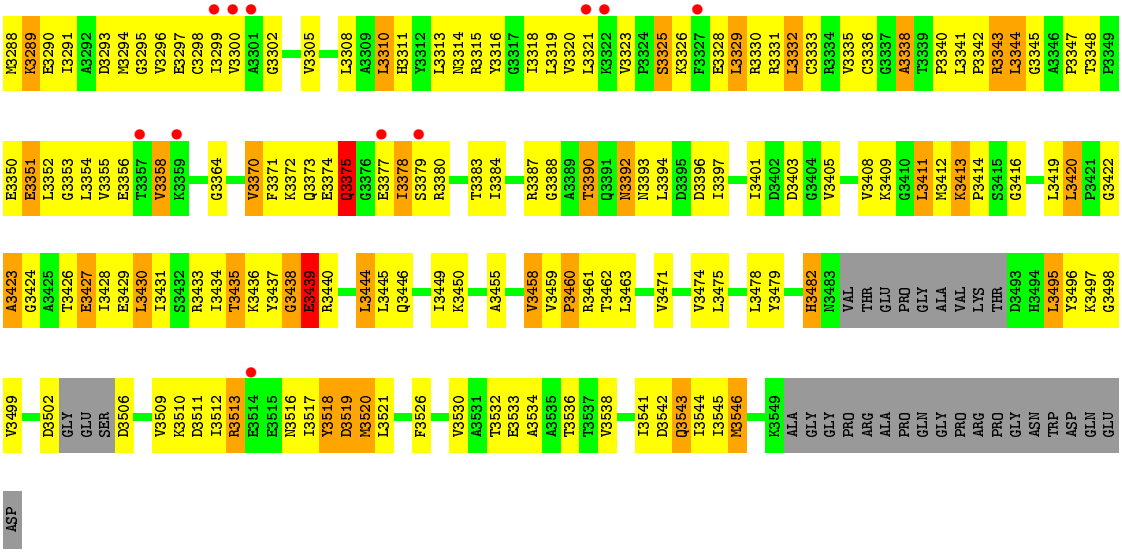
Chain Aq:



• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

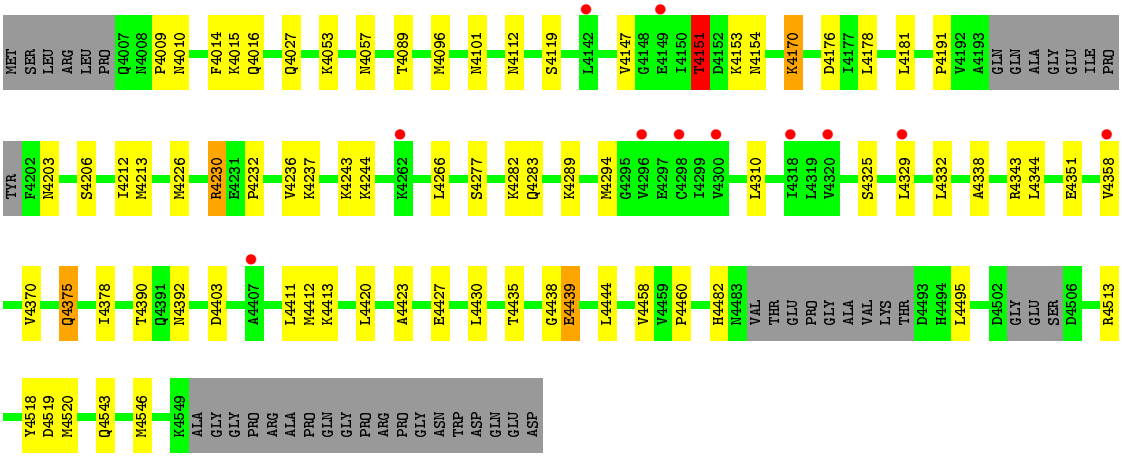
Chain BQ:





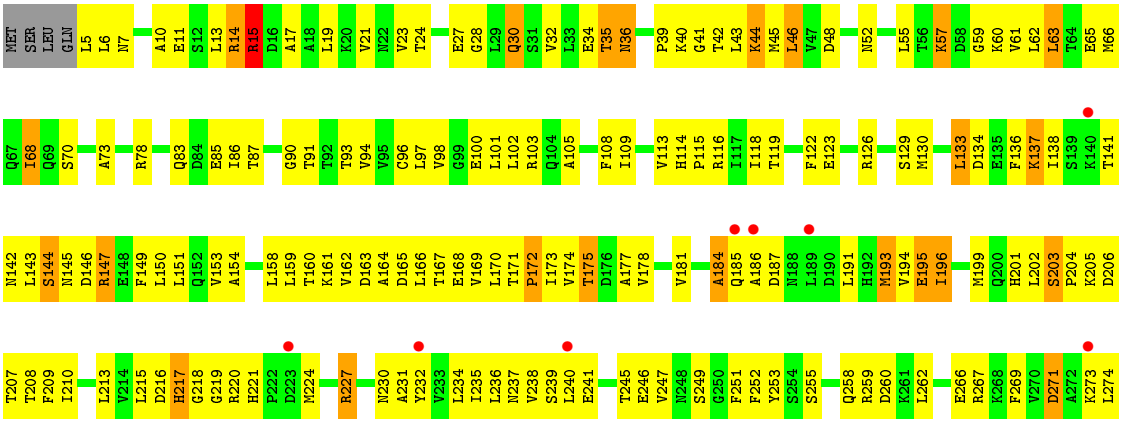
• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

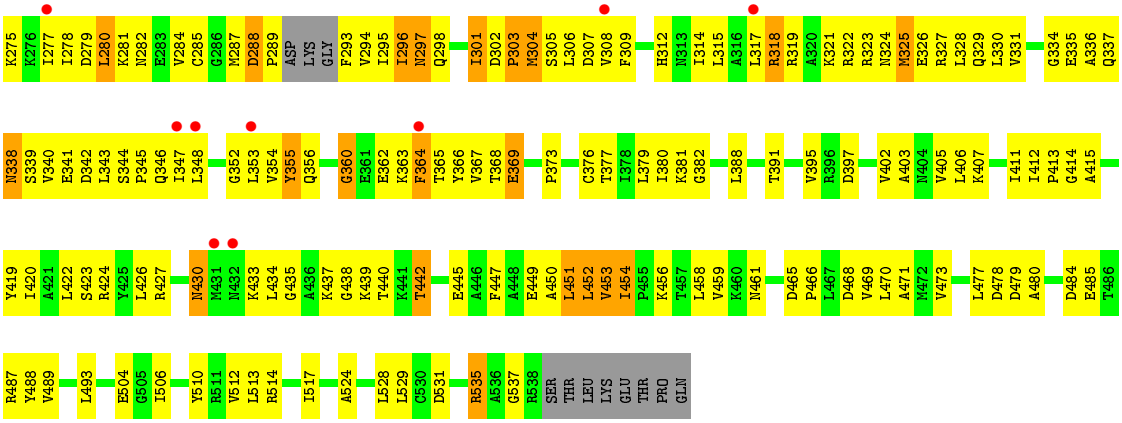
Chain Bq:

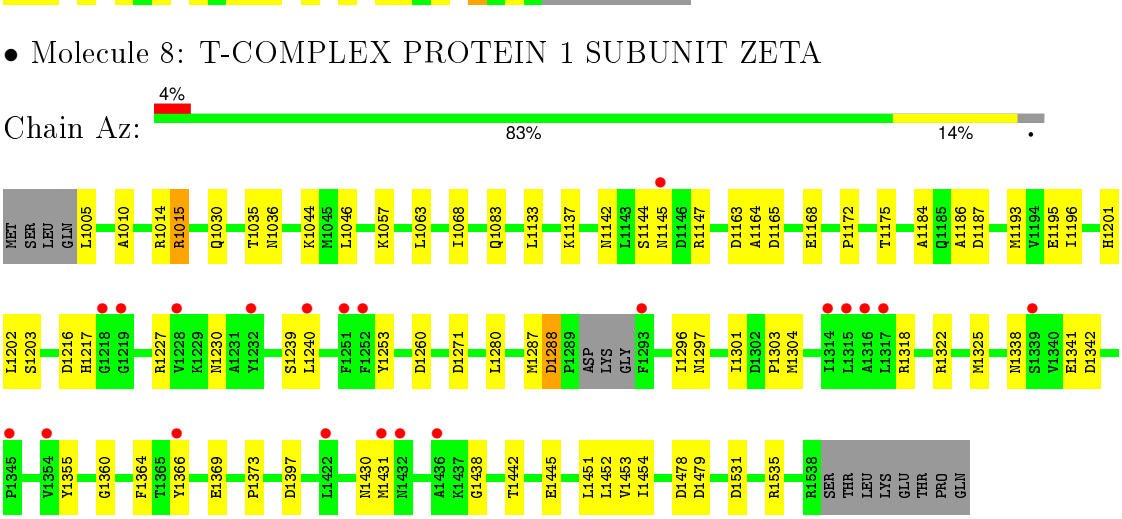


• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA

Chain AZ:





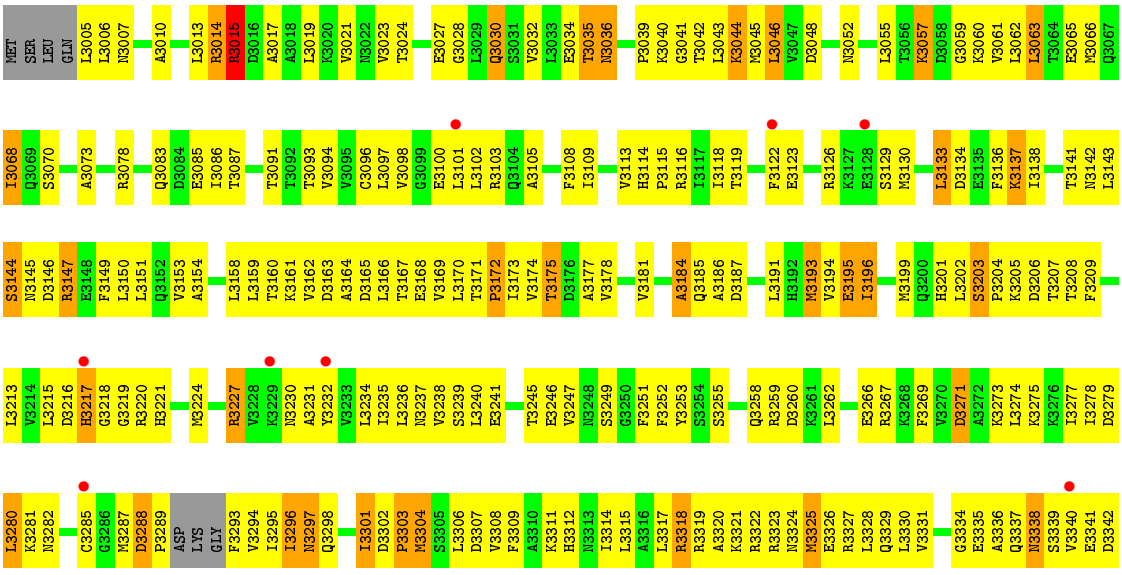


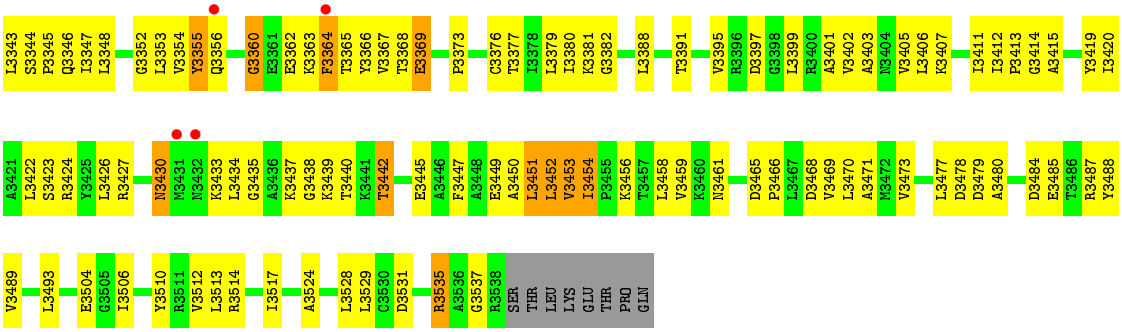
• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA

Chain Az:

• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA

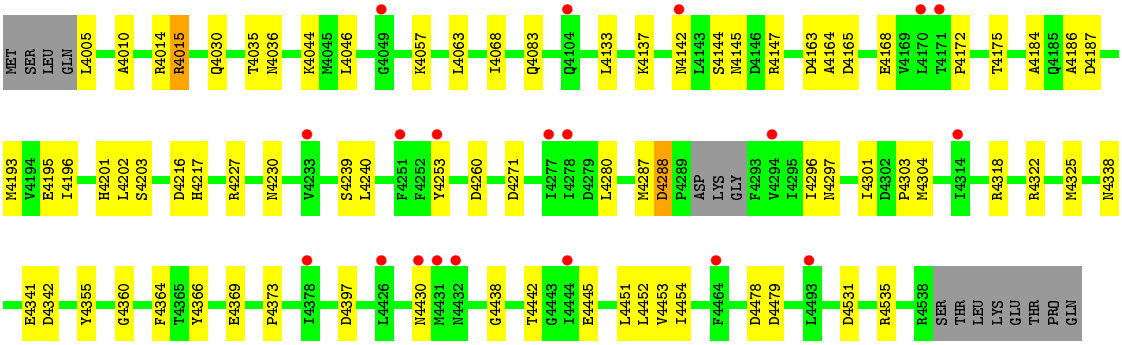
Chain BZ:





- Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA

Chain Bz:



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)	91.5 (89.95-3.80) 91.2 (89.95-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.78Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.248 , 0.284 0.248 , 0.281	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)	0.31 , 121.3	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	0.91	EDS
Total number of atoms	128780	wwPDB-VP
Average B, all atoms (Å^2)	131.0	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: MG, BEF, 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	AA	0.64	0/4095	0.78	2/5521 (0.0%)
1	Aa	0.64	0/4095	0.78	2/5521 (0.0%)
1	BA	0.64	0/4095	0.78	2/5521 (0.0%)
1	Ba	0.64	0/4095	0.78	2/5521 (0.0%)
2	AB	0.69	0/3966	0.80	1/5344 (0.0%)
2	Ab	0.69	0/3966	0.80	1/5344 (0.0%)
2	BB	0.69	0/3966	0.80	1/5344 (0.0%)
2	Bb	0.69	0/3966	0.80	1/5344 (0.0%)
3	AD	0.61	0/3974	0.77	1/5355 (0.0%)
3	Ad	0.61	0/3974	0.77	1/5355 (0.0%)
3	BD	0.61	0/3974	0.77	1/5355 (0.0%)
3	Bd	0.61	0/3974	0.77	1/5355 (0.0%)
4	AE	0.67	0/4117	0.78	2/5539 (0.0%)
4	Ae	0.67	0/4117	0.78	2/5539 (0.0%)
4	BE	0.67	0/4117	0.78	2/5539 (0.0%)
4	Be	0.67	0/4117	0.78	2/5539 (0.0%)
5	AG	0.60	0/3957	0.74	0/5340
5	Ag	0.60	0/3957	0.74	0/5340
5	BG	0.60	0/3957	0.74	0/5340
5	Bg	0.60	0/3957	0.74	0/5340
6	AH	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
6	Ah	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
6	BH	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
6	Bh	0.66	1/4010 (0.0%)	0.78	2/5412 (0.0%)
7	AQ	0.62	0/4025	0.75	1/5426 (0.0%)
7	Aq	0.62	0/4025	0.75	1/5426 (0.0%)
7	BQ	0.62	0/4025	0.75	1/5426 (0.0%)
7	Bq	0.62	0/4025	0.75	1/5426 (0.0%)
8	AZ	0.65	0/4140	0.72	0/5594
8	Az	0.65	0/4140	0.72	0/5594
8	BZ	0.65	0/4140	0.72	0/5594
8	Bz	94.13	3/4140 (0.1%)	1.43	3/5594 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	16.87	7/129136 (0.0%)	0.80	39/174124 (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
8	AZ	0	1
8	Az	0	1
8	BZ	0	1
8	Bz	0	1
All	All	0	4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Bz	4287	MET	CG-SD	4418.85	116.70	1.81
8	Bz	4287	MET	CB-CG	3613.95	117.16	1.51
8	Bz	4287	MET	SD-CE	2023.56	115.09	1.77
6	BH	3010	ILE	CA-CB	5.25	1.67	1.54
6	AH	10	ILE	CA-CB	5.25	1.67	1.54

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Bz	4287	MET	CG-SD-CE	-61.94	1.09	100.20
8	Bz	4287	MET	CA-CB-CG	-57.26	15.96	113.30
8	Bz	4287	MET	CB-CG-SD	-37.01	1.38	112.40
3	BD	3017	PRO	N-CA-C	-7.14	93.54	112.10
3	AD	17	PRO	N-CA-C	-7.14	93.55	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	AZ	366	TYR	Sidechain
8	Az	1366	TYR	Sidechain
8	BZ	3366	TYR	Sidechain
8	Bz	4366	TYR	Sidechain

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	AA	4060	0	4220	345	0
1	Aa	4060	0	4220	0	0
1	BA	4060	0	4220	343	0
1	Ba	4060	0	4220	0	0
2	AB	3927	0	4030	361	0
2	Ab	3927	0	4030	0	0
2	BB	3927	0	4030	353	0
2	Bb	3927	0	4030	0	0
3	AD	3938	0	4109	292	0
3	Ad	3938	0	4109	0	0
3	BD	3938	0	4109	294	0
3	Bd	3938	0	4109	0	0
4	AE	4068	0	4163	363	5
4	Ae	4068	0	4163	0	0
4	BE	4068	0	4163	359	2
4	Be	4068	0	4163	0	0
5	AG	3914	0	4057	297	0
5	Ag	3914	0	4057	0	0
5	BG	3914	0	4057	295	0
5	Bg	3914	0	4057	0	1
6	AH	3962	0	4045	357	0
6	Ah	3962	0	4045	0	1
6	BH	3962	0	4045	351	0
6	Bh	3962	0	4045	0	5
7	AQ	3981	0	4120	319	1
7	Aq	3981	0	4120	0	0
7	BQ	3981	0	4120	319	0
7	Bq	3981	0	4120	0	2
8	AZ	4089	0	4183	307	0
8	Az	4089	0	4183	0	1
8	BZ	4089	0	4183	302	0
8	Bz	4089	0	4183	0	0
9	AA	27	0	12	1	0
9	AB	27	0	12	2	0
9	AD	27	0	12	4	0
9	AE	27	0	12	2	0
9	AG	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AH	27	0	12	0	0
9	AQ	27	0	12	1	0
9	AZ	27	0	12	3	0
9	Aa	27	0	12	0	0
9	Ab	27	0	12	0	0
9	Ad	27	0	12	0	0
9	Ae	27	0	12	0	0
9	Ag	27	0	12	0	0
9	Ah	27	0	12	0	0
9	Aq	27	0	12	0	0
9	Az	27	0	12	0	0
9	BA	27	0	12	1	0
9	BB	27	0	12	2	0
9	BD	27	0	12	4	0
9	BE	27	0	12	2	0
9	BG	27	0	12	2	0
9	BH	27	0	12	0	0
9	BQ	27	0	12	1	0
9	BZ	27	0	12	2	0
9	Ba	27	0	12	0	0
9	Bb	27	0	12	0	0
9	Bd	27	0	12	0	0
9	Be	27	0	12	0	0
9	Bg	27	0	12	0	0
9	Bh	27	0	12	0	0
9	Bq	27	0	12	0	0
9	Bz	27	0	12	0	0
10	AA	4	0	0	0	0
10	AB	4	0	0	0	0
10	AD	4	0	0	0	0
10	AE	4	0	0	0	0
10	AG	4	0	0	2	0
10	AH	4	0	0	0	0
10	AQ	4	0	0	0	0
10	AZ	4	0	0	0	0
10	Aa	4	0	0	0	0
10	Ab	4	0	0	0	0
10	Ad	4	0	0	0	0
10	Ae	4	0	0	0	0
10	Ag	4	0	0	0	0
10	Ah	4	0	0	0	0
10	Aq	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Az	4	0	0	0	0
10	BA	4	0	0	0	0
10	BB	4	0	0	0	0
10	BD	4	0	0	0	0
10	BE	4	0	0	0	0
10	BG	4	0	0	2	0
10	BH	4	0	0	0	0
10	BQ	4	0	0	0	0
10	BZ	4	0	0	0	0
10	Ba	4	0	0	0	0
10	Bb	4	0	0	0	0
10	Bd	4	0	0	0	0
10	Be	4	0	0	0	0
10	Bg	4	0	0	0	0
10	Bh	4	0	0	0	0
10	Bq	4	0	0	0	0
10	Bz	4	0	0	0	0
11	AA	1	0	0	0	0
11	AB	1	0	0	0	0
11	AD	1	0	0	0	0
11	AE	1	0	0	0	0
11	AG	1	0	0	0	0
11	AH	1	0	0	0	0
11	AQ	1	0	0	0	0
11	AZ	1	0	0	0	0
11	Aa	1	0	0	0	0
11	Ab	1	0	0	0	0
11	Ad	1	0	0	0	0
11	Ae	1	0	0	0	0
11	Ag	1	0	0	0	0
11	Ah	1	0	0	0	0
11	Aq	1	0	0	0	0
11	Az	1	0	0	0	0
11	BA	1	0	0	0	0
11	BB	1	0	0	0	0
11	BD	1	0	0	0	0
11	BE	1	0	0	0	0
11	BG	1	0	0	0	0
11	BH	1	0	0	0	0
11	BQ	1	0	0	0	0
11	BZ	1	0	0	0	0
11	Ba	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Bb	1	0	0	0	0
11	Bd	1	0	0	0	0
11	Be	1	0	0	0	0
11	Bg	1	0	0	0	0
11	Bh	1	0	0	0	0
11	Bq	1	0	0	0	0
11	Bz	1	0	0	0	0
All	All	128780	0	132092	4783	9

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 37.

The worst 5 of 4783 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)
4:BE:3413:LYS:HE3	4:BE:3413:LYS:H	1.17	1.09
7:BQ:3257:ALA:HB2	7:BQ:3343:ARG:HH22	1.18	1.08
3:AD:141:LYS:HA	3:AD:409:GLY:HA2	1.39	1.05
7:AQ:257:ALA:HB2	7:AQ:343:ARG:HH22	1.18	1.03
4:AE:413:LYS:HE3	4:AE:413:LYS:H	1.17	1.03

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AE:462:ARG:CD	6:Bh:4151:LYS:CE[1_465]	1.74	0.46
4:AE:460:LYS:N	6:Bh:4149:SER:O[1_465]	1.81	0.39
4:BE:3174:GLU:OE2	7:Bq:4151:THR:CB[1_465]	1.88	0.32
4:AE:462:ARG:CD	6:Bh:4151:LYS:CD[1_465]	2.01	0.19
7:AQ:514:GLU:OE2	6:Ah:1151:LYS:NZ[1_465]	2.10	0.10

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	AA	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1 20
1	Aa	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1 20
1	BA	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1 20
1	Ba	531/559 (95%)	388 (73%)	103 (19%)	40 (8%)	1 20
2	AB	515/527 (98%)	382 (74%)	100 (19%)	33 (6%)	2 26
2	Ab	515/527 (98%)	383 (74%)	99 (19%)	33 (6%)	2 26
2	BB	515/527 (98%)	382 (74%)	100 (19%)	33 (6%)	2 26
2	Bb	515/527 (98%)	382 (74%)	100 (19%)	33 (6%)	2 26
3	AD	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1 24
3	Ad	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1 24
3	BD	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1 24
3	Bd	511/528 (97%)	391 (76%)	85 (17%)	35 (7%)	1 24
4	AE	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1 25
4	Ae	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1 25
4	BE	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1 25
4	Be	526/562 (94%)	401 (76%)	91 (17%)	34 (6%)	1 25
5	AG	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2 26
5	Ag	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2 26
5	BG	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2 26
5	Bg	503/590 (85%)	387 (77%)	85 (17%)	31 (6%)	2 26
6	AH	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1 22
6	Ah	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1 22
6	BH	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1 22
6	Bh	517/550 (94%)	389 (75%)	91 (18%)	37 (7%)	1 22
7	AQ	515/568 (91%)	415 (81%)	73 (14%)	27 (5%)	2 30
7	Aq	515/568 (91%)	414 (80%)	74 (14%)	27 (5%)	2 30
7	BQ	515/568 (91%)	414 (80%)	74 (14%)	27 (5%)	2 30
7	Bq	515/568 (91%)	415 (81%)	73 (14%)	27 (5%)	2 30
8	AZ	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2 31
8	Az	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2 31
8	BZ	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	Bz	527/546 (96%)	403 (76%)	97 (18%)	27 (5%)	2 31
All	All	16580/17720 (94%)	12623 (76%)	2901 (18%)	1056 (6%)	2 26

5 of 1056 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	77	HIS
1	AA	335	ALA
1	AA	378	SER
2	AB	5	ILE
2	AB	15	ALA

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	AA	450/471 (96%)	393 (87%)	57 (13%)	5 32
1	Aa	450/471 (96%)	393 (87%)	57 (13%)	5 32
1	BA	450/471 (96%)	393 (87%)	57 (13%)	5 32
1	Ba	450/471 (96%)	393 (87%)	57 (13%)	5 32
2	AB	431/441 (98%)	363 (84%)	68 (16%)	3 23
2	Ab	431/441 (98%)	363 (84%)	68 (16%)	3 23
2	BB	431/441 (98%)	363 (84%)	68 (16%)	3 23
2	Bb	431/441 (98%)	363 (84%)	68 (16%)	3 23
3	AD	443/454 (98%)	388 (88%)	55 (12%)	6 33
3	Ad	443/454 (98%)	388 (88%)	55 (12%)	6 33
3	BD	443/454 (98%)	388 (88%)	55 (12%)	6 33
3	Bd	443/454 (98%)	388 (88%)	55 (12%)	6 33
4	AE	454/483 (94%)	404 (89%)	50 (11%)	8 39
4	Ae	454/483 (94%)	404 (89%)	50 (11%)	8 39
4	BE	454/483 (94%)	404 (89%)	50 (11%)	8 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	Be	454/483 (94%)	404 (89%)	50 (11%)	8 39
5	AG	433/497 (87%)	379 (88%)	54 (12%)	6 33
5	Ag	433/497 (87%)	379 (88%)	54 (12%)	6 33
5	BG	433/497 (87%)	379 (88%)	54 (12%)	6 33
5	Bg	433/497 (87%)	379 (88%)	54 (12%)	6 33
6	AH	430/454 (95%)	379 (88%)	51 (12%)	6 35
6	Ah	430/454 (95%)	379 (88%)	51 (12%)	6 35
6	BH	430/454 (95%)	379 (88%)	51 (12%)	6 35
6	Bh	430/454 (95%)	379 (88%)	51 (12%)	6 35
7	AQ	439/473 (93%)	387 (88%)	52 (12%)	6 35
7	Aq	439/473 (93%)	387 (88%)	52 (12%)	6 35
7	BQ	439/473 (93%)	387 (88%)	52 (12%)	6 35
7	Bq	439/473 (93%)	387 (88%)	52 (12%)	6 35
8	AZ	449/463 (97%)	399 (89%)	50 (11%)	8 39
8	Az	449/463 (97%)	399 (89%)	50 (11%)	8 39
8	BZ	449/463 (97%)	399 (89%)	50 (11%)	8 39
8	Bz	449/463 (97%)	400 (89%)	49 (11%)	8 40
All	All	14116/14944 (94%)	12369 (88%)	1747 (12%)	6 33

5 of 1747 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	Aq	1226	MET
2	BB	3337	LEU
6	Bh	4231	GLN
7	Aq	1435	THR
1	BA	3142	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 464 such sidechains are listed below:

Mol	Chain	Res	Type
7	Aq	1203	ASN
3	BD	3112	ASN
6	Bh	4436	GLN
7	Aq	1543	GLN

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Mol	Chain	Res	Type
1	BA	3225	ASN

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 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 for Mogul analysis.

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	AA	601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.41	4 (14%)
10	BEF	AA	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AB	601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.28	4 (14%)
10	BEF	AB	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AD	601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.71	5 (18%)
10	BEF	AD	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AE	601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.39	4 (14%)
10	BEF	AE	602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AG	1001	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.22	3 (11%)
10	BEF	AG	1002	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AH	601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.36	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BEF	AH	602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AQ	601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.56	5 (18%)
10	BEF	AQ	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	AZ	601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.46	5 (18%)
10	BEF	AZ	602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Aa	1601	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.41	4 (14%)
10	BEF	Aa	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ab	1601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.28	4 (14%)
10	BEF	Ab	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ad	1601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.72	6 (22%)
10	BEF	Ad	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ae	1601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.39	4 (14%)
10	BEF	Ae	1602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ag	2001	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.21	3 (11%)
10	BEF	Ag	2002	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ah	1601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.35	4 (14%)
10	BEF	Ah	1602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Aq	1601	11,10	22,29,29	2.23	5 (22%)	27,45,45	3.55	5 (18%)
10	BEF	Aq	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Az	1601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.47	5 (18%)
10	BEF	Az	1602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BA	3601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.42	4 (14%)
10	BEF	BA	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BB	3601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.29	4 (14%)
10	BEF	BB	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BD	3601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.72	5 (18%)
10	BEF	BD	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BE	3601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.39	4 (14%)
10	BEF	BE	3602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BG	4001	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.22	3 (11%)
10	BEF	BG	4002	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BH	3601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.35	4 (14%)
10	BEF	BH	3602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BQ	3601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.56	5 (18%)
10	BEF	BQ	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	BZ	3601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.47	5 (18%)
10	BEF	BZ	3602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Ba	4601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.40	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BEF	Ba	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bb	4601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.29	4 (14%)
10	BEF	Bb	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bd	4601	11,10	22,29,29	2.25	5 (22%)	27,45,45	3.71	5 (18%)
10	BEF	Bd	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Be	4601	11,10	22,29,29	2.27	5 (22%)	27,45,45	3.40	4 (14%)
10	BEF	Be	4602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bg	5001	11,10	22,29,29	2.28	5 (22%)	27,45,45	3.23	3 (11%)
10	BEF	Bg	5002	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bh	4601	11,10	22,29,29	2.24	5 (22%)	27,45,45	3.36	4 (14%)
10	BEF	Bh	4602	9,11	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bq	4601	11,10	22,29,29	2.22	5 (22%)	27,45,45	3.49	3 (11%)
10	BEF	Bq	4602	9	0,3,3	0.00	-	0,3,3	0.00	-
9	ADP	Bz	4601	11,10	22,29,29	2.26	5 (22%)	27,45,45	3.46	5 (18%)
10	BEF	Bz	4602	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	AA	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AA	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AB	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AB	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AD	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AD	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AE	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AE	602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	AG	1001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AG	1002	9	-	0/0/0/0	0/0/0/0
9	ADP	AH	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AH	602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	AQ	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AQ	602	9	-	0/0/0/0	0/0/0/0
9	ADP	AZ	601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	AZ	602	9	-	0/0/0/0	0/0/0/0
9	ADP	Aa	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Aa	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ab	1601	11,10	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BEF	Ab	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ad	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ad	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ae	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ae	1602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Ag	2001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ag	2002	9	-	0/0/0/0	0/0/0/0
9	ADP	Ah	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ah	1602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Aq	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Aq	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	Az	1601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Az	1602	9	-	0/0/0/0	0/0/0/0
9	ADP	BA	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BA	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BB	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BB	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BD	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BD	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BE	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BE	3602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	BG	4001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BG	4002	9	-	0/0/0/0	0/0/0/0
9	ADP	BH	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BH	3602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	BQ	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BQ	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	BZ	3601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	BZ	3602	9	-	0/0/0/0	0/0/0/0
9	ADP	Ba	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Ba	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Bb	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bb	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Bd	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bd	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Be	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Be	4602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Bg	5001	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bg	5002	9	-	0/0/0/0	0/0/0/0
9	ADP	Bh	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bh	4602	9,11	-	0/0/0/0	0/0/0/0
9	ADP	Bq	4601	11,10	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BEF	Bq	4602	9	-	0/0/0/0	0/0/0/0
9	ADP	Bz	4601	11,10	-	0/12/32/32	0/3/3/3
10	BEF	Bz	4602	9	-	0/0/0/0	0/0/0/0

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AQ	601	ADP	C5-C4	-2.95	1.33	1.40
9	Aq	1601	ADP	C5-C4	-2.94	1.33	1.40
9	Be	4601	ADP	C5-C4	-2.94	1.33	1.40
9	Ae	1601	ADP	C5-C4	-2.92	1.33	1.40
9	AE	601	ADP	C5-C4	-2.92	1.33	1.40

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Be	4601	ADP	N3-C2-N1	-16.31	116.41	128.89
9	BE	3601	ADP	N3-C2-N1	-16.28	116.43	128.89
9	AE	601	ADP	N3-C2-N1	-16.27	116.43	128.89
9	Ae	1601	ADP	N3-C2-N1	-16.26	116.44	128.89
9	Bh	4601	ADP	N3-C2-N1	-16.16	116.52	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AA	601	ADP	1	0
9	AB	601	ADP	2	0
9	AD	601	ADP	4	0
9	AE	601	ADP	2	0
9	AG	1001	ADP	2	0
10	AG	1002	BEF	2	0
9	AQ	601	ADP	1	0
9	AZ	601	ADP	3	0
9	BA	3601	ADP	1	0
9	BB	3601	ADP	2	0
9	BD	3601	ADP	4	0
9	BE	3601	ADP	2	0
9	BG	4001	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	BG	4002	BEF	2	0
9	BQ	3601	ADP	1	0
9	BZ	3601	ADP	2	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	AA	537/559 (96%)	0.14	6 (1%) 82 69	71, 129, 176, 248	0
1	Aa	537/559 (96%)	0.12	8 (1%) 76 62	71, 129, 176, 248	0
1	BA	537/559 (96%)	0.07	5 (0%) 85 74	71, 129, 176, 248	0
1	Ba	537/559 (96%)	0.15	15 (2%) 56 40	71, 129, 176, 248	0
2	AB	517/527 (98%)	0.11	7 (1%) 78 63	58, 112, 163, 205	0
2	Ab	517/527 (98%)	0.04	6 (1%) 81 67	58, 112, 163, 205	0
2	BB	517/527 (98%)	0.07	3 (0%) 90 82	58, 112, 163, 205	0
2	Bb	517/527 (98%)	0.08	9 (1%) 73 58	58, 112, 163, 205	0
3	AD	515/528 (97%)	0.19	8 (1%) 74 60	60, 128, 174, 224	0
3	Ad	515/528 (97%)	0.36	22 (4%) 39 25	60, 128, 174, 224	0
3	BD	515/528 (97%)	0.09	6 (1%) 81 67	60, 128, 174, 224	0
3	Bd	515/528 (97%)	0.20	15 (2%) 55 38	60, 128, 174, 224	0
4	AE	528/562 (93%)	0.08	4 (0%) 87 77	63, 121, 173, 218	0
4	Ae	528/562 (93%)	0.18	14 (2%) 58 42	63, 121, 173, 218	0
4	BE	528/562 (93%)	0.08	3 (0%) 90 82	63, 121, 173, 218	0
4	Be	528/562 (93%)	0.07	6 (1%) 82 69	63, 121, 173, 218	0
5	AG	509/590 (86%)	0.24	12 (2%) 62 46	78, 131, 179, 233	0
5	Ag	509/590 (86%)	0.32	15 (2%) 55 38	78, 131, 179, 233	0
5	BG	509/590 (86%)	0.24	14 (2%) 56 40	78, 131, 179, 233	0
5	Bg	509/590 (86%)	0.15	11 (2%) 65 50	78, 131, 179, 233	0
6	AH	519/550 (94%)	0.13	7 (1%) 79 65	66, 131, 173, 244	0
6	Ah	519/550 (94%)	0.21	16 (3%) 52 36	66, 131, 173, 244	0
6	BH	519/550 (94%)	0.18	6 (1%) 81 67	66, 131, 173, 244	0
6	Bh	519/550 (94%)	0.28	24 (4%) 36 24	66, 131, 173, 244	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
7	AQ	523/568 (92%)	0.15	5 (0%)	84	72	71, 138, 182, 249	0
7	Aq	523/568 (92%)	0.32	21 (4%)	42	28	71, 138, 182, 249	0
7	BQ	523/568 (92%)	0.26	18 (3%)	49	34	71, 138, 182, 249	0
7	Bq	523/568 (92%)	0.20	11 (2%)	67	51	71, 138, 182, 249	0
8	AZ	531/546 (97%)	0.24	17 (3%)	51	35	79, 135, 185, 261	0
8	Az	531/546 (97%)	0.21	21 (3%)	42	28	79, 135, 185, 261	0
8	BZ	531/546 (97%)	0.27	12 (2%)	64	48	79, 135, 185, 261	0
8	Bz	531/546 (97%)	0.24	20 (3%)	44	30	79, 135, 185, 261	0
All	All	16716/17720 (94%)	0.18	367 (2%)	65	50	58, 129, 177, 261	0

The worst 5 of 367 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ba	4488	LYS	9.6
8	Bz	4432	ASN	8.5
8	Az	1431	MET	7.3
8	Bz	4431	MET	6.7
8	Az	1316	ALA	6.7

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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	Ag	2002	4/4	0.92	0.31	1.48	154,176,182,188	0
10	BEF	Ba	4602	4/4	0.97	0.19	0.53	72,141,146,155	0
10	BEF	AG	1002	4/4	0.87	0.28	0.33	154,176,182,188	0
10	BEF	BB	3602	4/4	0.98	0.23	0.29	85,91,123,141	0
11	MG	BD	3603	1/1	0.92	0.23	0.20	78,78,78,78	0
10	BEF	Bh	4602	4/4	0.92	0.23	0.19	96,148,149,170	0
9	ADP	Ag	2001	27/27	0.94	0.30	0.09	66,124,161,173	0
9	ADP	BG	4001	27/27	0.94	0.28	-0.00	66,124,161,173	0
10	BEF	Ab	1602	4/4	0.98	0.22	-0.03	85,91,123,141	0
11	MG	AA	603	1/1	0.99	0.22	-0.07	117,117,117,117	0
10	BEF	Bb	4602	4/4	0.97	0.22	-0.08	85,91,123,141	0
9	ADP	AG	1001	27/27	0.94	0.28	-0.12	66,124,161,173	0
9	ADP	Ba	4601	27/27	0.96	0.24	-0.18	32,114,157,179	0
9	ADP	BB	3601	27/27	0.97	0.25	-0.19	55,93,132,149	0
11	MG	Ba	4603	1/1	0.99	0.18	-0.20	117,117,117,117	0
9	ADP	Ab	1601	27/27	0.96	0.24	-0.20	55,93,132,149	0
9	ADP	BD	3601	27/27	0.93	0.22	-0.20	78,119,143,177	0
9	ADP	AA	601	27/27	0.93	0.26	-0.21	32,114,157,179	0
9	ADP	Ae	1601	27/27	0.95	0.25	-0.21	30,104,142,184	0
11	MG	Ad	1603	1/1	0.95	0.25	-0.25	78,78,78,78	0
10	BEF	AD	602	4/4	0.98	0.21	-0.27	103,113,151,153	0
9	ADP	Bh	4601	27/27	0.97	0.25	-0.27	29,118,145,160	0
9	ADP	Bb	4601	27/27	0.96	0.24	-0.30	55,93,132,149	0
9	ADP	AH	601	27/27	0.94	0.27	-0.32	29,118,145,160	0
9	ADP	AE	601	27/27	0.96	0.22	-0.33	30,104,142,184	0
10	BEF	AQ	602	4/4	0.96	0.21	-0.33	154,160,163,170	0
10	BEF	Bq	4602	4/4	0.96	0.21	-0.36	154,160,163,170	0
11	MG	Aq	1603	1/1	0.98	0.28	-0.37	117,117,117,117	0
9	ADP	BE	3601	27/27	0.96	0.21	-0.38	30,104,142,184	0
11	MG	Bq	4603	1/1	0.96	0.21	-0.39	117,117,117,117	0
10	BEF	BE	3602	4/4	0.97	0.20	-0.40	109,121,145,150	0
9	ADP	Ah	1601	27/27	0.96	0.26	-0.46	29,118,145,160	0
9	ADP	Aa	1601	27/27	0.95	0.24	-0.50	32,114,157,179	0
10	BEF	AE	602	4/4	0.96	0.22	-0.50	109,121,145,150	0
9	ADP	Bq	4601	27/27	0.94	0.23	-0.51	55,126,167,172	0
11	MG	AG	1003	1/1	0.94	0.25	-0.52	117,117,117,117	0
9	ADP	AD	601	27/27	0.95	0.23	-0.54	78,119,143,177	0
10	BEF	Ae	1602	4/4	0.95	0.21	-0.58	109,121,145,150	0
9	ADP	AB	601	27/27	0.98	0.25	-0.62	55,93,132,149	0
10	BEF	BA	3602	4/4	0.97	0.21	-0.64	72,141,146,155	0
9	ADP	Be	4601	27/27	0.96	0.20	-0.67	30,104,142,184	0
11	MG	AD	603	1/1	0.99	0.18	-0.69	78,78,78,78	0
9	ADP	Bg	5001	27/27	0.94	0.21	-0.74	66,124,161,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	BEF	Ah	1602	4/4	0.98	0.17	-0.75	96,148,149,170	0
9	ADP	BQ	3601	27/27	0.96	0.21	-0.76	55,126,167,172	0
9	ADP	Az	1601	27/27	0.95	0.20	-0.78	91,121,146,151	0
9	ADP	Bz	4601	27/27	0.95	0.21	-0.78	91,121,146,151	0
11	MG	BQ	3603	1/1	0.92	0.20	-0.78	117,117,117,117	0
10	BEF	BG	4002	4/4	0.95	0.18	-0.81	154,176,182,188	0
9	ADP	AQ	601	27/27	0.95	0.25	-0.82	55,126,167,172	0
9	ADP	BZ	3601	27/27	0.94	0.22	-0.84	91,121,146,151	0
9	ADP	Ad	1601	27/27	0.94	0.18	-0.84	78,119,143,177	0
10	BEF	BD	3602	4/4	0.98	0.15	-0.87	103,113,151,153	0
11	MG	Aa	1603	1/1	0.99	0.20	-0.93	117,117,117,117	0
10	BEF	Bg	5002	4/4	0.91	0.21	-0.95	154,176,182,188	0
9	ADP	BA	3601	27/27	0.96	0.20	-0.96	32,114,157,179	0
9	ADP	BH	3601	27/27	0.97	0.21	-0.98	29,118,145,160	0
10	BEF	Be	4602	4/4	0.98	0.17	-0.98	109,121,145,150	0
10	BEF	Bz	4602	4/4	0.92	0.15	-1.01	100,122,147,169	0
10	BEF	AA	602	4/4	0.96	0.15	-1.08	72,141,146,155	0
9	ADP	Bd	4601	27/27	0.97	0.21	-1.11	78,119,143,177	0
10	BEF	AB	602	4/4	0.99	0.21	-1.12	85,91,123,141	0
10	BEF	AH	602	4/4	0.92	0.19	-1.14	96,148,149,170	0
9	ADP	Aq	1601	27/27	0.96	0.20	-1.15	55,126,167,172	0
10	BEF	Az	1602	4/4	0.97	0.17	-1.24	100,122,147,169	0
9	ADP	AZ	601	27/27	0.96	0.20	-1.24	91,121,146,151	0
10	BEF	BH	3602	4/4	0.99	0.15	-1.24	96,148,149,170	0
10	BEF	BZ	3602	4/4	0.94	0.21	-1.27	100,122,147,169	0
10	BEF	BQ	3602	4/4	0.96	0.17	-1.27	154,160,163,170	0
10	BEF	Aa	1602	4/4	0.96	0.17	-1.31	72,141,146,155	0
10	BEF	Bd	4602	4/4	0.97	0.20	-1.34	103,113,151,153	0
11	MG	Bd	4603	1/1	0.99	0.17	-1.51	78,78,78,78	0
11	MG	BG	4003	1/1	0.91	0.15	-1.59	117,117,117,117	0
11	MG	AQ	603	1/1	0.97	0.15	-1.65	117,117,117,117	0
10	BEF	Aq	1602	4/4	0.98	0.10	-1.72	154,160,163,170	0
11	MG	BA	3603	1/1	0.99	0.17	-1.74	117,117,117,117	0
10	BEF	Ad	1602	4/4	0.95	0.11	-1.94	103,113,151,153	0
10	BEF	AZ	602	4/4	0.98	0.16	-1.98	100,122,147,169	0
11	MG	Ag	2003	1/1	0.98	0.18	-3.95	117,117,117,117	0
11	MG	Bg	5003	1/1	0.94	0.15	-4.66	117,117,117,117	0
11	MG	AH	603	1/1	0.99	0.23	-	112,112,112,112	0
11	MG	Be	4603	1/1	0.95	0.21	-	88,88,88,88	0
11	MG	AZ	603	1/1	0.98	0.13	-	96,96,96,96	0
11	MG	BE	3603	1/1	0.99	0.15	-	88,88,88,88	0
11	MG	BB	3603	1/1	0.95	0.28	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	MG	Bz	4603	1/1	0.96	0.15	-	96,96,96,96	0
11	MG	Bh	4603	1/1	0.99	0.10	-	112,112,112,112	0
11	MG	Az	1603	1/1	0.94	0.18	-	96,96,96,96	0
11	MG	Ah	1603	1/1	0.98	0.19	-	112,112,112,112	0
11	MG	BH	3603	1/1	0.97	0.14	-	112,112,112,112	0
11	MG	Ab	1603	1/1	0.96	0.26	-	79,79,79,79	0
11	MG	Bb	4603	1/1	0.98	0.20	-	79,79,79,79	0
11	MG	AE	603	1/1	0.99	0.21	-	88,88,88,88	0
11	MG	BZ	3603	1/1	0.97	0.12	-	96,96,96,96	0
11	MG	AB	603	1/1	0.99	0.18	-	79,79,79,79	0
11	MG	Ae	1603	1/1	0.96	0.19	-	88,88,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.