



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:00 PM GMT

PDB ID : 4B2T
Title : The crystal structures of the eukaryotic chaperonin CCT reveal its functional partitioning
Authors : Kalisman, N.; Schroeder, G.F.; Levitt, M.
Deposited on : 2012-07-17
Resolution : 5.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

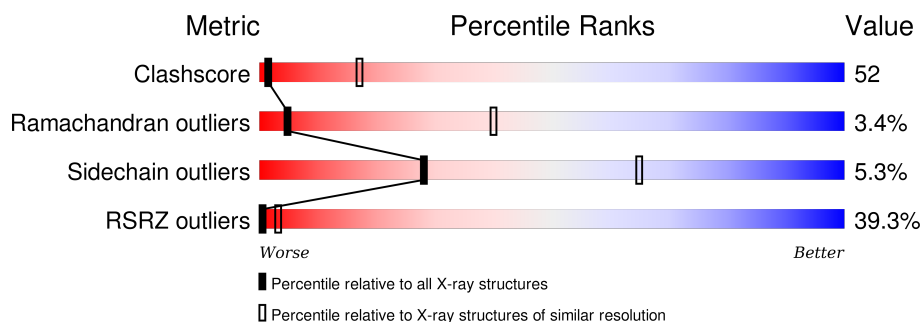
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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))
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	<div> <div>26%</div> <div>29%</div> <div>51%</div> <div>6%</div> <div>13%</div> </div>
1	a	556	<div> <div>29%</div> <div>57%</div> <div>6%</div> <div>35%</div> </div>
2	B	535	<div> <div>44%</div> <div>35%</div> <div>52%</div> <div>10%</div> </div>
2	b	535	<div> <div>31%</div> <div>62%</div> <div>5%</div> <div>33%</div> </div>
3	D	542	<div> <div>31%</div> <div>28%</div> <div>55%</div> <div>5%</div> <div>11%</div> </div>
3	d	542	<div> <div>26%</div> <div>61%</div> <div>5%</div> <div>34%</div> </div>
4	E	541	<div> <div>22%</div> <div>32%</div> <div>50%</div> <div>7%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
4	e	541	
5	G	545	
5	g	545	
6	H	543	
6	h	543	
7	Q	548	
7	q	548	
8	Z	531	
8	z	531	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 51877 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	481	Total	C	N	O	S	0	0	0
			3625	2280	633	692	20			
1	a	359	Total	C	N	O	S	0	0	0
			2705	1703	469	520	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	481	Total	C	N	O	S	0	0	0
			3602	2258	629	696	19			
2	b	359	Total	C	N	O	S	0	0	0
			2658	1652	469	524	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	481	Total	C	N	O	S	0	0	0
			3610	2259	627	703	21			
3	d	359	Total	C	N	O	S	0	0	0
			2690	1671	473	532	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	158	VAL	GLU	CONFLICT	UNP Q2T9X2
D	510	LEU	GLN	CONFLICT	UNP Q2T9X2
d	1158	VAL	GLU	CONFLICT	UNP Q2T9X2
d	1510	LEU	GLN	CONFLICT	UNP Q2T9X2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	481	Total	C	N	O	S	0	0	0
			3674	2299	644	703	28			
4	e	359	Total	C	N	O	S	0	0	0
			2724	1688	486	528	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	481	Total	C	N	O	S	0	0	0
			3719	2326	661	705	27			
5	g	359	Total	C	N	O	S	0	0	0
			2735	1711	480	523	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	481	Total	C	N	O	S	0	0	0
			3671	2320	633	693	25			
6	h	359	Total	C	N	O	S	0	0	0
			2724	1719	472	517	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Q	481	Total	C	N	O	S	0	0	0
			3673	2317	628	703	25			
7	q	359	Total	C	N	O	S	0	0	0
			2739	1729	467	526	17			

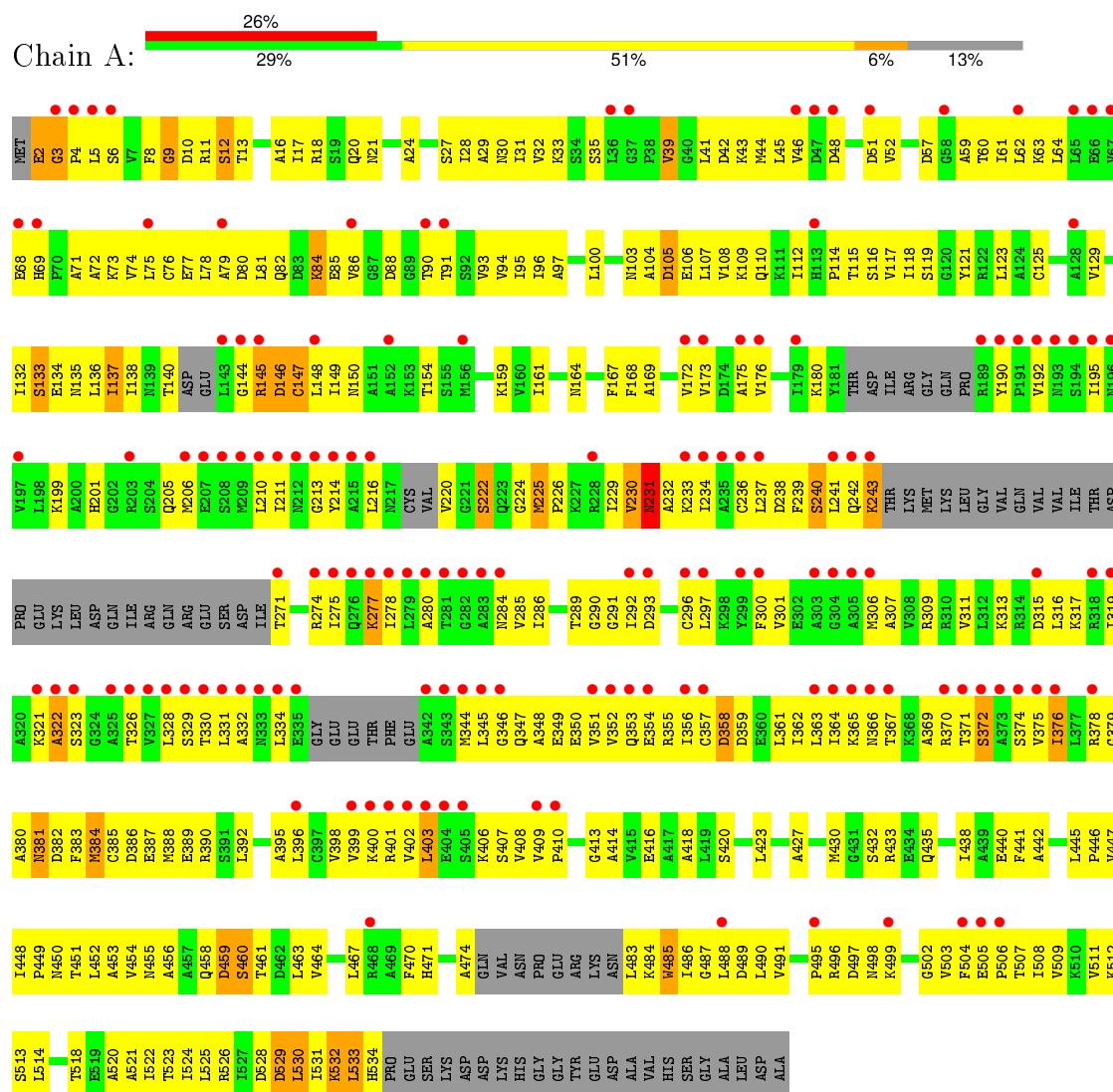
- Molecule 8 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ZETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Z	481	Total	C	N	O	S	0	0	0
			3664	2310	638	697	19			
8	z	481	Total	C	N	O	S	0	0	0
			3664	2310	638	697	19			

3 Residue-property plots

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.

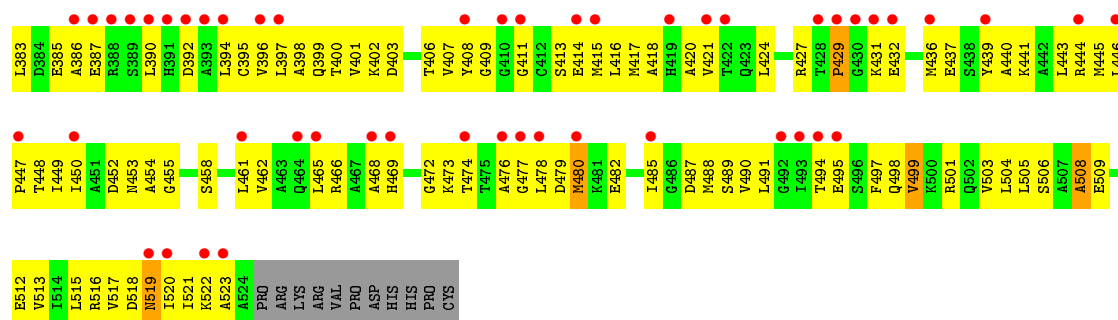
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA



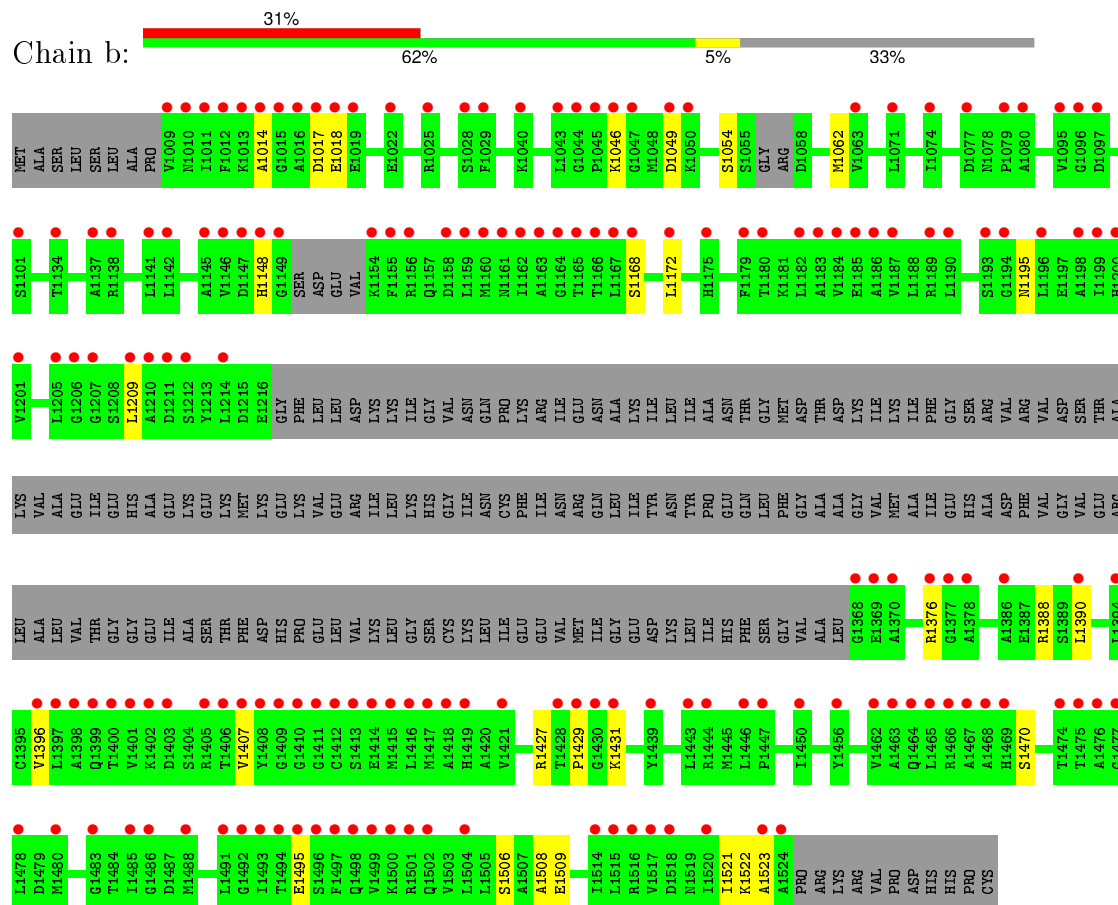
• Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA



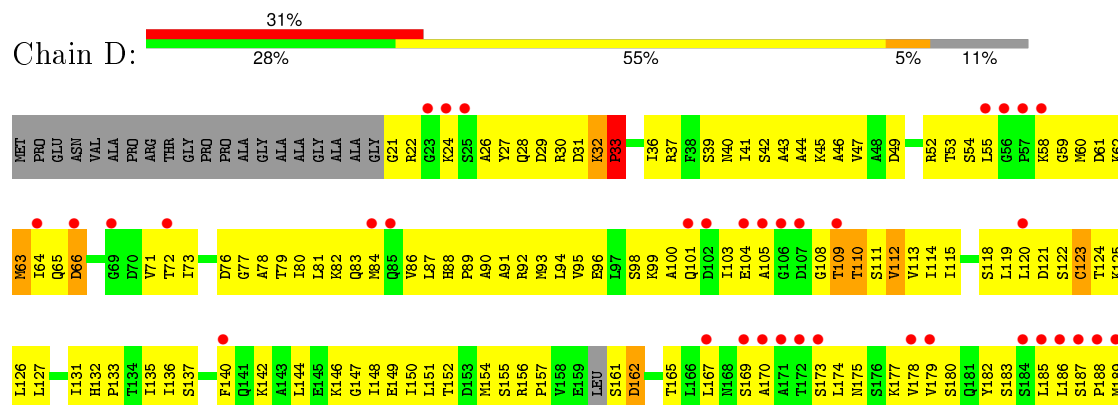


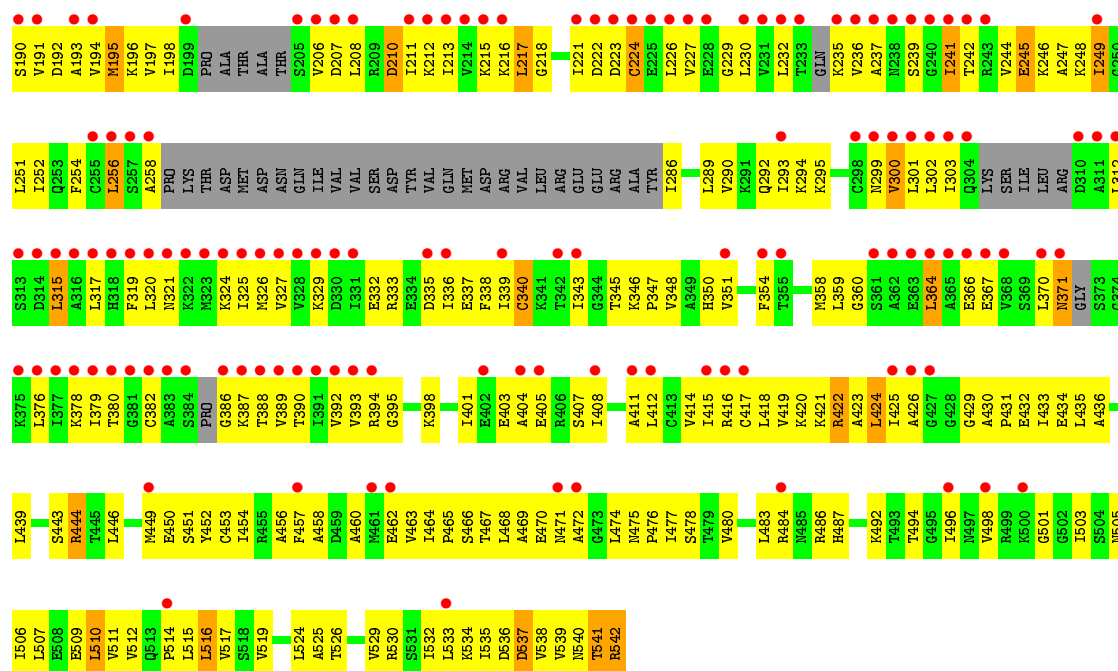


• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

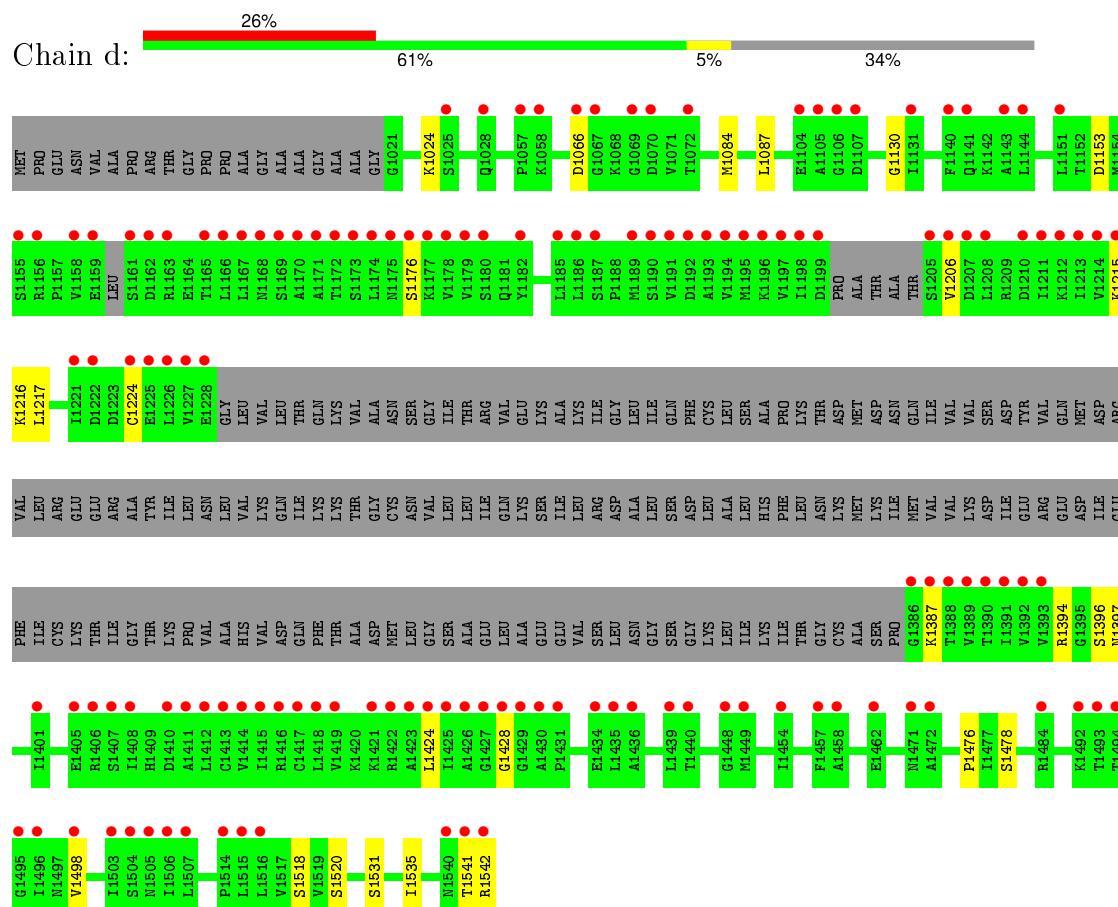


• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA





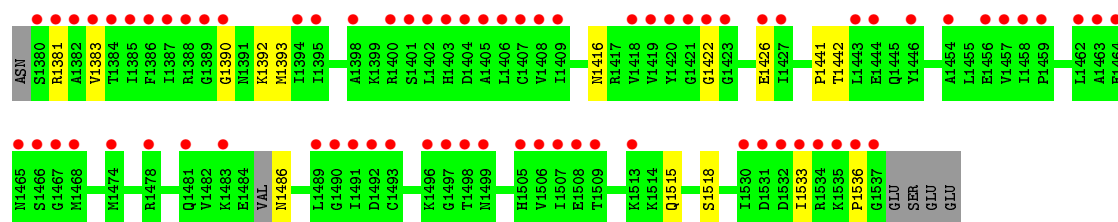
• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA



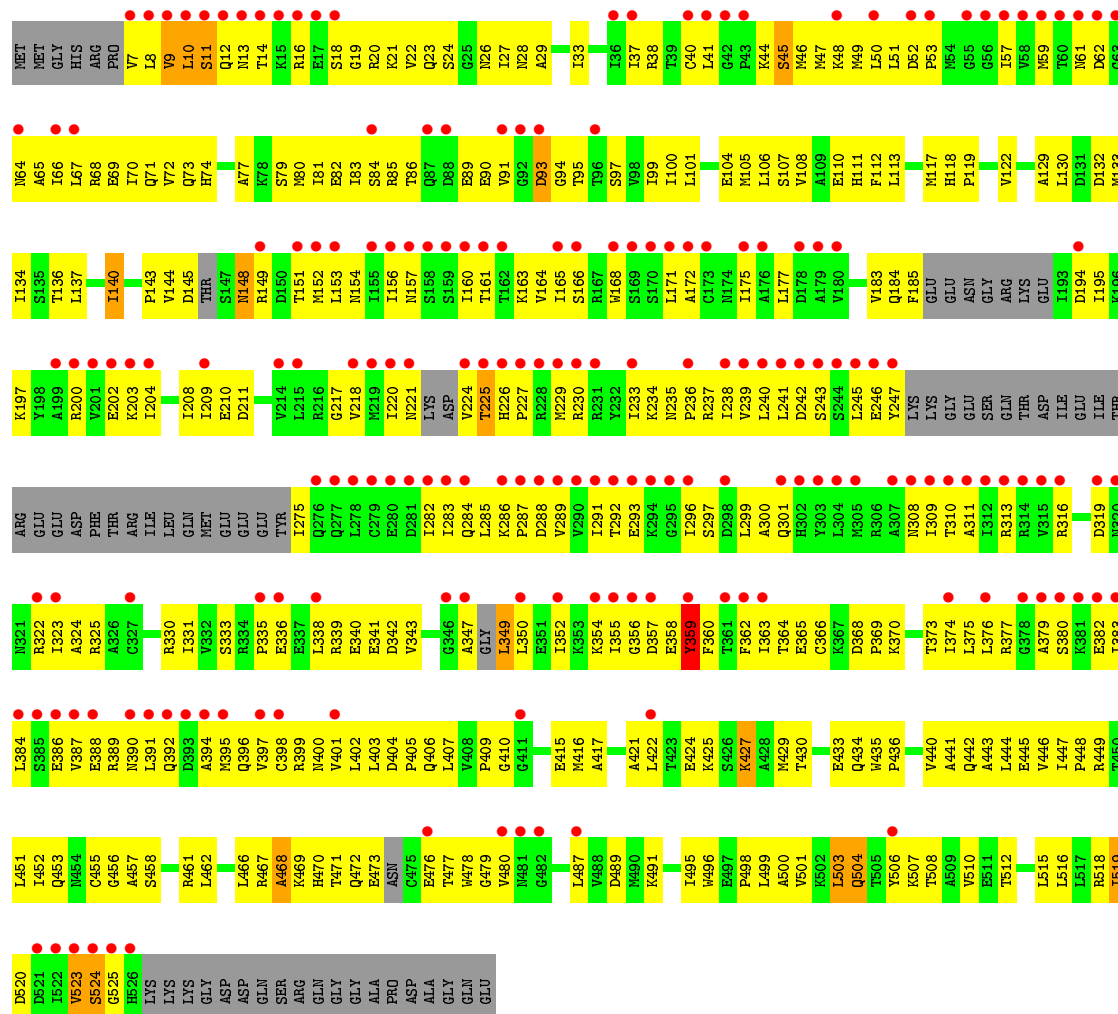
• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON





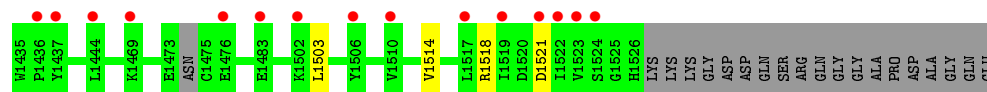


● Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

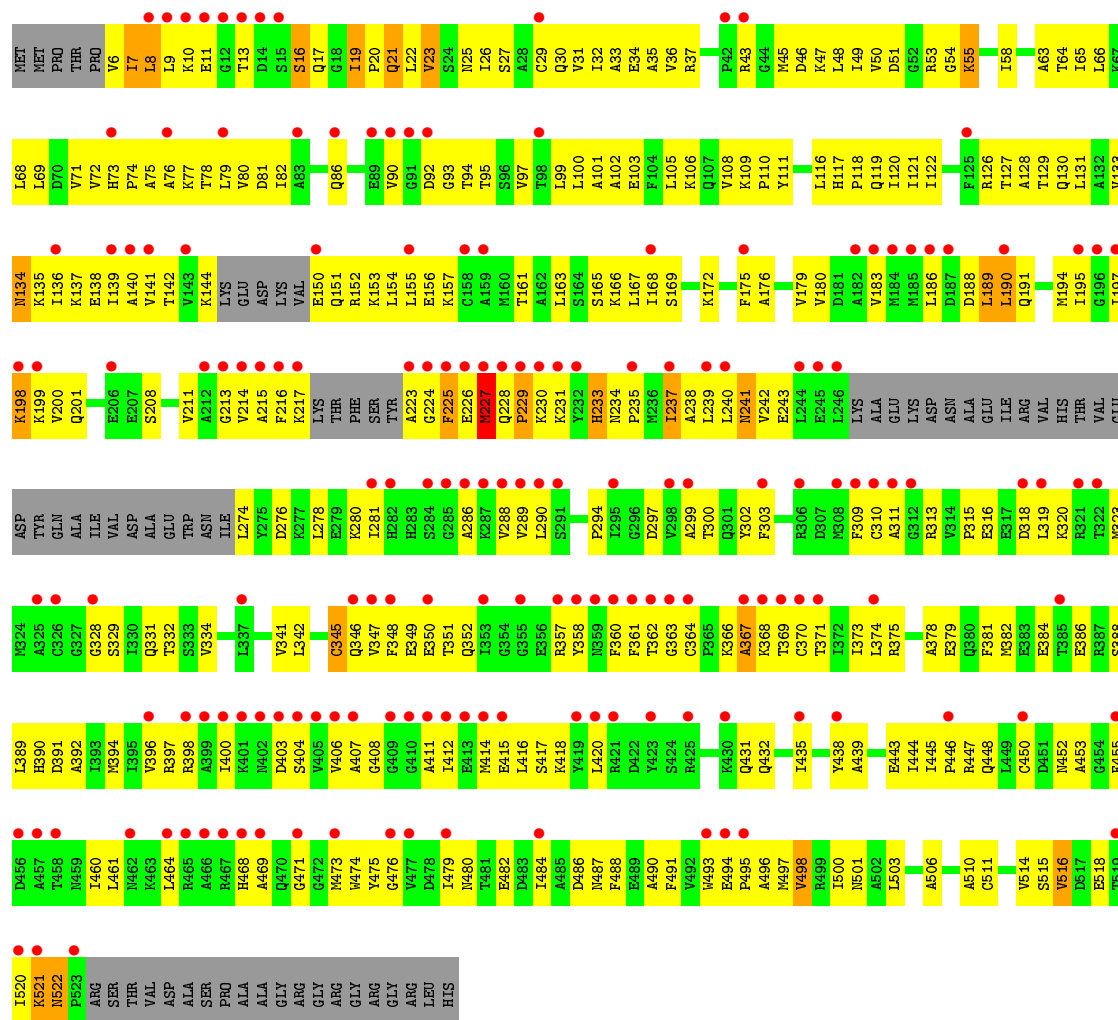


● Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA



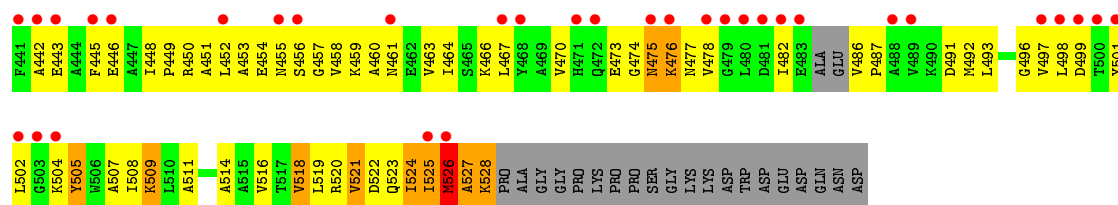


• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

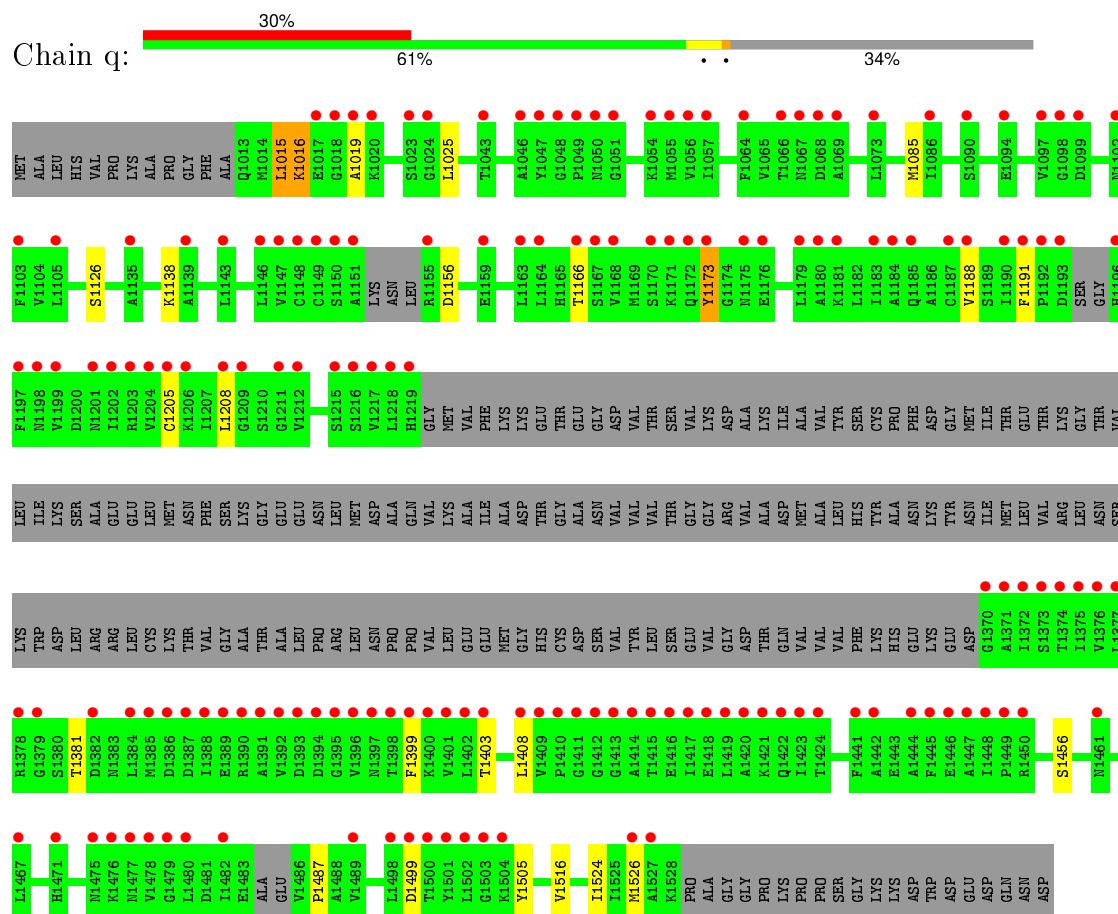


- Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

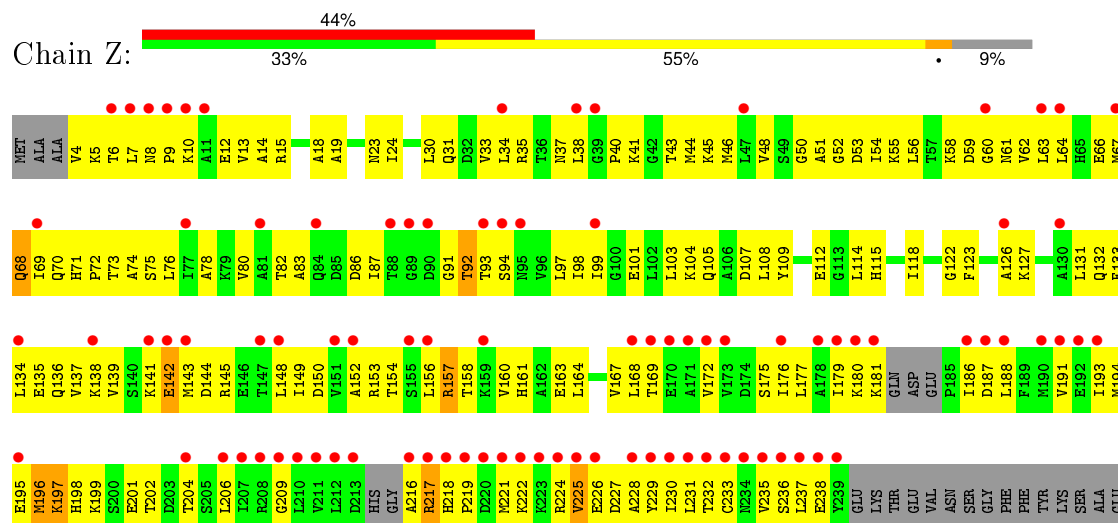


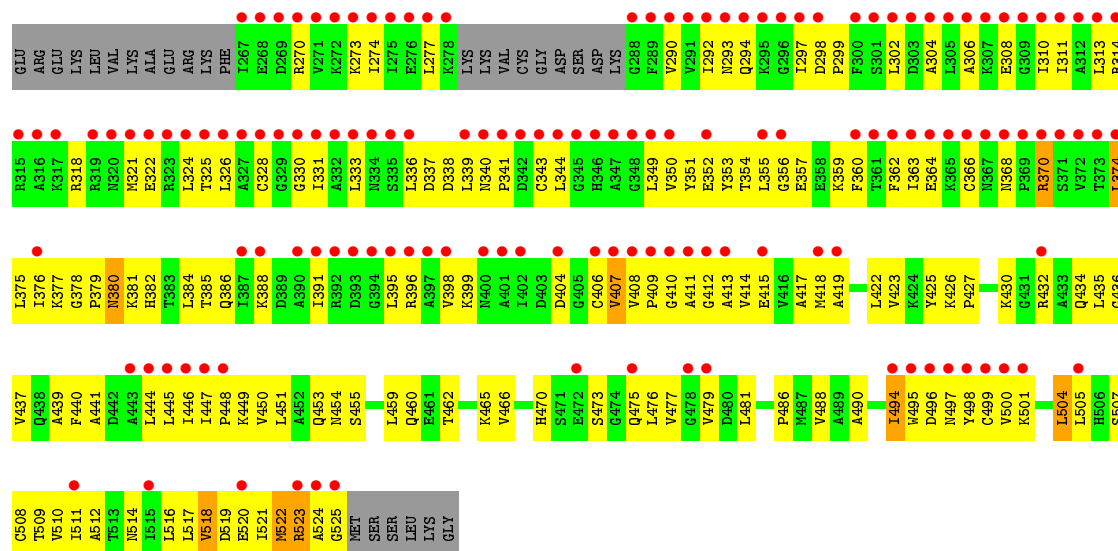


• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

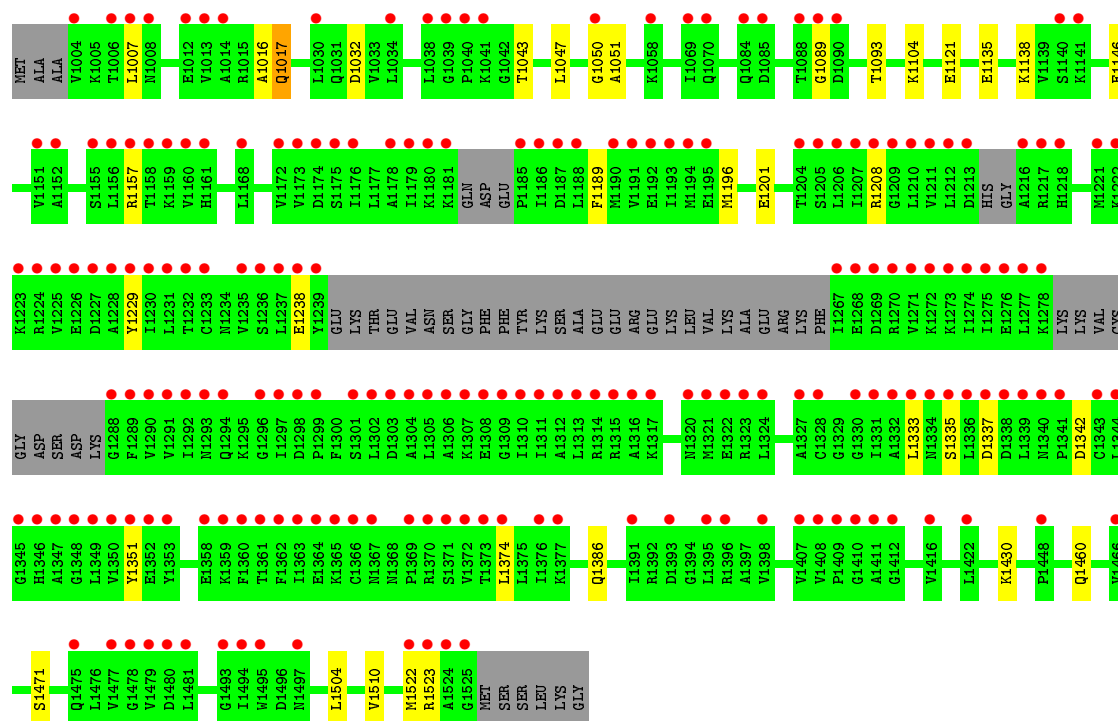
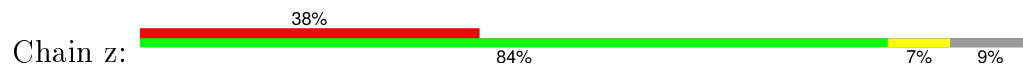


• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA





● Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	272.70 Å 313.50 Å 158.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 5.50 97.58 – 5.44	Depositor EDS
% Data completeness (in resolution range)	99.1 (200.00-5.50) 98.4 (97.58-5.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 5.41 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.340 , 0.399 0.328 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	257.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 427.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 45495 reflections	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	51877	wwPDB-VP
Average B, all atoms (Å ²)	277.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/3657	0.44	0/4934
1	a	0.22	0/2733	0.46	0/3695
2	B	0.22	0/3638	0.43	0/4903
2	b	0.21	0/2680	0.44	0/3615
3	D	0.21	0/3632	0.46	0/4891
3	d	0.21	0/2707	0.45	0/3650
4	E	0.22	0/3712	0.44	0/4997
4	e	0.21	0/2743	0.44	0/3687
5	G	0.21	0/3758	0.45	0/5073
5	g	0.21	0/2763	0.46	0/3733
6	H	0.23	0/3716	0.43	0/5008
6	h	0.22	0/2751	0.45	0/3711
7	Q	0.23	0/3724	0.44	0/5032
7	q	0.23	0/2774	0.43	0/3746
8	Z	0.22	0/3702	0.44	0/4995
8	z	0.21	0/3702	0.45	0/4995
All	All	0.22	0/52392	0.44	0/70665

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	3625	0	3783	380	0
1	a	2705	0	2799	0	0
2	B	3602	0	3705	353	0
2	b	2658	0	2733	0	0
3	D	3610	0	3810	456	0
3	d	2690	0	2818	0	0
4	E	3674	0	3781	382	0
4	e	2724	0	2822	0	0
5	G	3719	0	3870	398	0
5	g	2735	0	2851	0	0
6	H	3671	0	3783	366	0
6	h	2724	0	2842	0	0
7	Q	3673	0	3719	383	0
7	q	2739	0	2777	0	0
8	Z	3664	0	3820	413	0
8	z	3664	0	3820	0	0
All	All	51877	0	53733	2912	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 52.

The worst 5 of 2912 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)
5:G:456:GLY:HA3	8:Z:118:ILE:HD11	1.37	1.06
1:A:211:ILE:HG22	1:A:213:GLY:H	1.21	1.04
3:D:540:ASN:HB3	3:D:542:ARG:HD3	1.36	1.03
4:E:94:LEU:HD21	4:E:523:MET:HB2	1.39	1.03
7:Q:525:ILE:HG23	7:Q:526:MET:H	1.22	1.03

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	471/556 (85%)	390 (83%)	63 (13%)	18 (4%)	4	37
1	a	351/556 (63%)	283 (81%)	50 (14%)	18 (5%)	2	29
2	B	473/535 (88%)	398 (84%)	62 (13%)	13 (3%)	6	44
2	b	353/535 (66%)	301 (85%)	42 (12%)	10 (3%)	6	44
3	D	469/542 (86%)	385 (82%)	70 (15%)	14 (3%)	5	42
3	d	351/542 (65%)	300 (86%)	42 (12%)	9 (3%)	7	45
4	E	471/541 (87%)	392 (83%)	60 (13%)	19 (4%)	4	35
4	e	351/541 (65%)	295 (84%)	39 (11%)	17 (5%)	3	31
5	G	471/545 (86%)	396 (84%)	62 (13%)	13 (3%)	6	44
5	g	351/545 (64%)	291 (83%)	51 (14%)	9 (3%)	7	45
6	H	473/543 (87%)	384 (81%)	73 (15%)	16 (3%)	5	40
6	h	353/543 (65%)	289 (82%)	54 (15%)	10 (3%)	6	44
7	Q	473/548 (86%)	406 (86%)	45 (10%)	22 (5%)	3	32
7	q	351/548 (64%)	292 (83%)	48 (14%)	11 (3%)	5	42
8	Z	473/531 (89%)	400 (85%)	57 (12%)	16 (3%)	5	40
8	z	473/531 (89%)	403 (85%)	57 (12%)	13 (3%)	6	44
All	All	6708/8682 (77%)	5605 (84%)	875 (13%)	228 (3%)	5	40

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLY
1	A	145	ARG
1	A	146	ASP
1	A	230	VAL
2	B	54	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/461 (86%)	368 (93%)	27 (7%)	20	57
1	a	297/461 (64%)	269 (91%)	28 (9%)	11	42
2	B	382/429 (89%)	372 (97%)	10 (3%)	54	80
2	b	281/429 (66%)	263 (94%)	18 (6%)	22	59
3	D	407/454 (90%)	388 (95%)	19 (5%)	32	68
3	d	303/454 (67%)	285 (94%)	18 (6%)	24	61
4	E	400/455 (88%)	371 (93%)	29 (7%)	17	55
4	e	298/455 (66%)	283 (95%)	15 (5%)	30	66
5	G	416/470 (88%)	402 (97%)	14 (3%)	44	76
5	g	307/470 (65%)	288 (94%)	19 (6%)	23	60
6	H	394/445 (88%)	381 (97%)	13 (3%)	45	76
6	h	292/445 (66%)	274 (94%)	18 (6%)	23	60
7	Q	398/452 (88%)	380 (96%)	18 (4%)	34	69
7	q	296/452 (66%)	279 (94%)	17 (6%)	25	62
8	Z	398/440 (90%)	386 (97%)	12 (3%)	48	77
8	z	398/440 (90%)	374 (94%)	24 (6%)	24	61
All	All	5662/7212 (78%)	5363 (95%)	299 (5%)	28	65

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Z	370	ARG
1	a	1523	THR
8	z	1017	GLN
8	Z	508	CYS
1	a	1125	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
7	Q	435	GLN
1	a	1393	HIS
8	z	1070	GLN
8	Z	23	ASN
8	Z	453	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/556 (86%)	1.72	145 (30%) 1 4	260, 260, 260, 260	0
1	a	359/556 (64%)	2.23	159 (44%) 0 3	282, 282, 282, 282	0
2	B	481/535 (89%)	2.76	237 (49%) 0 3	281, 281, 281, 281	0
2	b	359/535 (67%)	2.33	167 (46%) 0 3	272, 272, 272, 272	0
3	D	481/542 (88%)	1.93	168 (34%) 0 3	289, 289, 289, 289	0
3	d	359/542 (66%)	1.92	139 (38%) 0 3	266, 266, 266, 266	0
4	E	481/541 (88%)	1.35	121 (25%) 1 4	262, 262, 262, 262	0
4	e	359/541 (66%)	2.55	170 (47%) 0 3	283, 283, 283, 283	0
5	G	481/545 (88%)	2.09	192 (39%) 0 3	283, 283, 283, 283	0
5	g	359/545 (65%)	1.27	86 (23%) 1 4	275, 275, 275, 275	0
6	H	481/543 (88%)	1.82	170 (35%) 0 3	272, 272, 272, 272	0
6	h	359/543 (66%)	1.29	98 (27%) 1 4	258, 258, 258, 258	0
7	Q	481/548 (87%)	2.74	241 (50%) 0 3	308, 308, 308, 308	0
7	q	359/548 (65%)	2.15	162 (45%) 0 3	261, 261, 261, 261	0
8	Z	481/531 (90%)	2.68	232 (48%) 0 3	297, 297, 297, 297	0
8	z	481/531 (90%)	2.51	201 (41%) 0 3	276, 276, 276, 276	0
All	All	6842/8682 (78%)	2.10	2688 (39%) 0 3	258, 276, 308, 308	0

The worst 5 of 2688 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	Z	288	GLY	26.2
8	z	1209	GLY	22.1
6	H	224	GLY	19.0
8	z	1288	GLY	17.1
4	e	1226	LYS	16.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.