



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:19 AM UTC

PDB ID : 4B2T / pdb_00004b2t
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

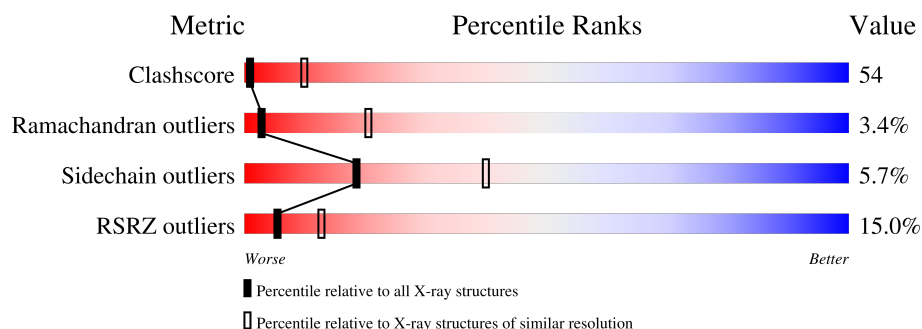
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	9% 27% 53% 6% 13%
1	a	556	13% 17% 42% 6% 35%
2	B	535	12% 34% 53% • 10%
2	b	535	9% 24% 39% • 33%
3	D	542	8% 27% 56% 6% 11%
3	d	542	12% 19% 44% • 34%
4	E	541	12% 30% 52% 6% 11%

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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.

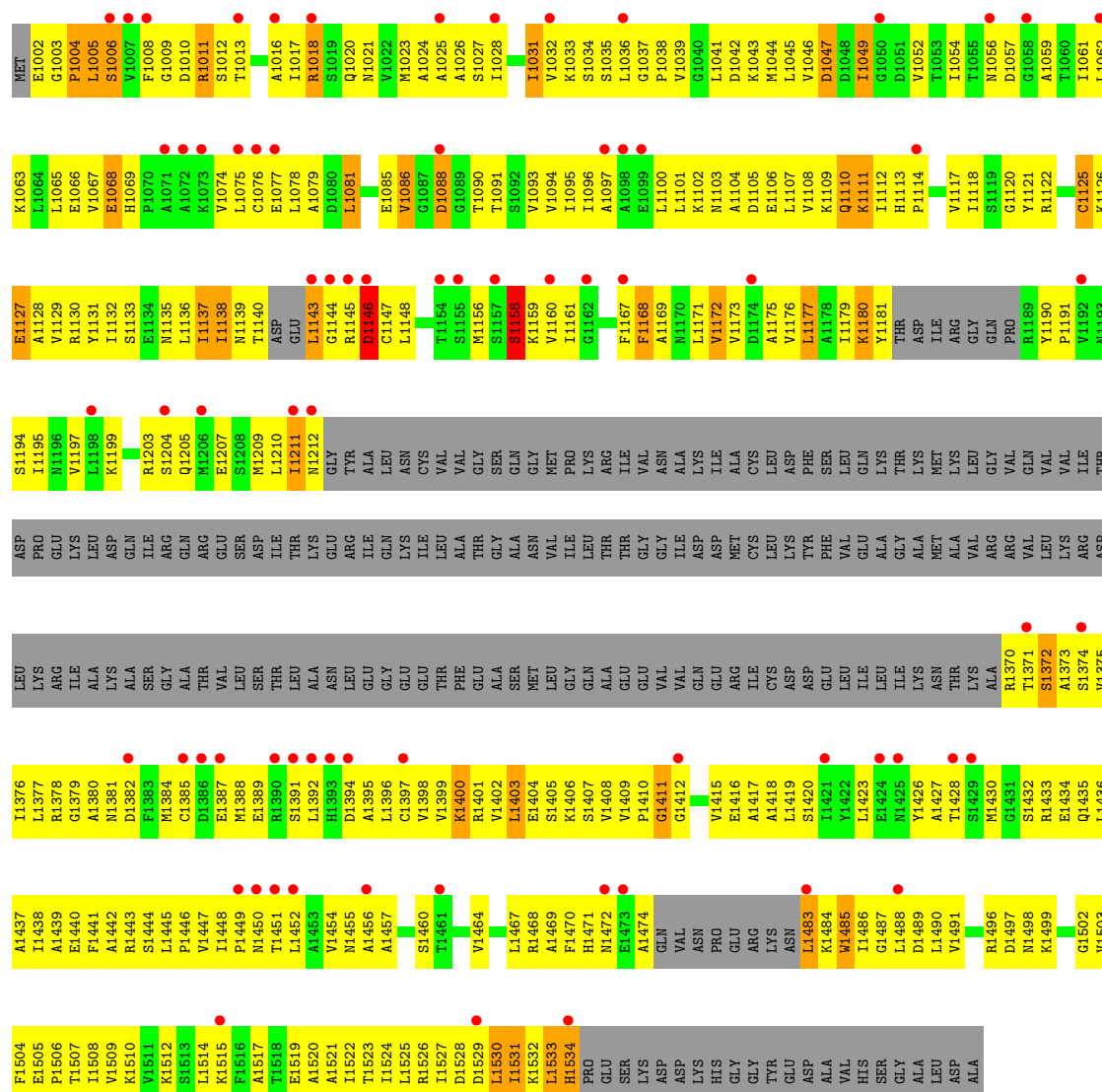
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	481	Total	C	N	O	S	0	0	0
			3671	2320	633	693	25			
6	h	359	Total	C	N	O	S	0	0	0
			2724	1719	472	517	16			

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

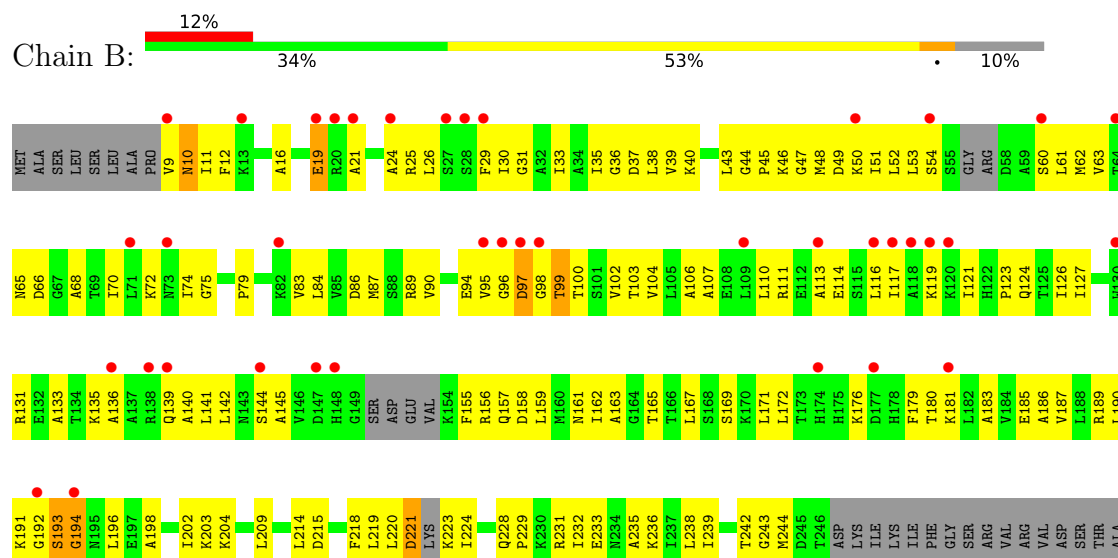
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Q	481	Total	C	N	O	S	0	0	0
			3673	2317	628	703	25			
7	q	359	Total	C	N	O	S	0	0	0
			2739	1729	467	526	17			

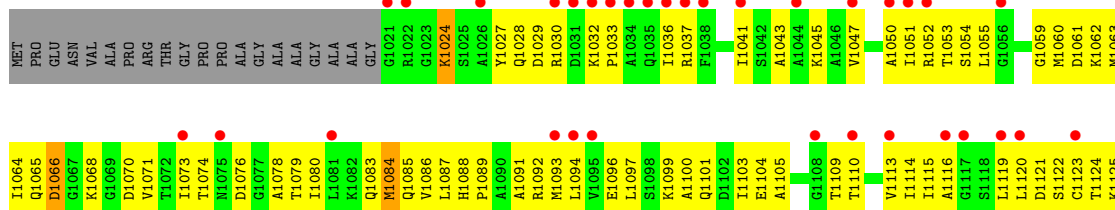
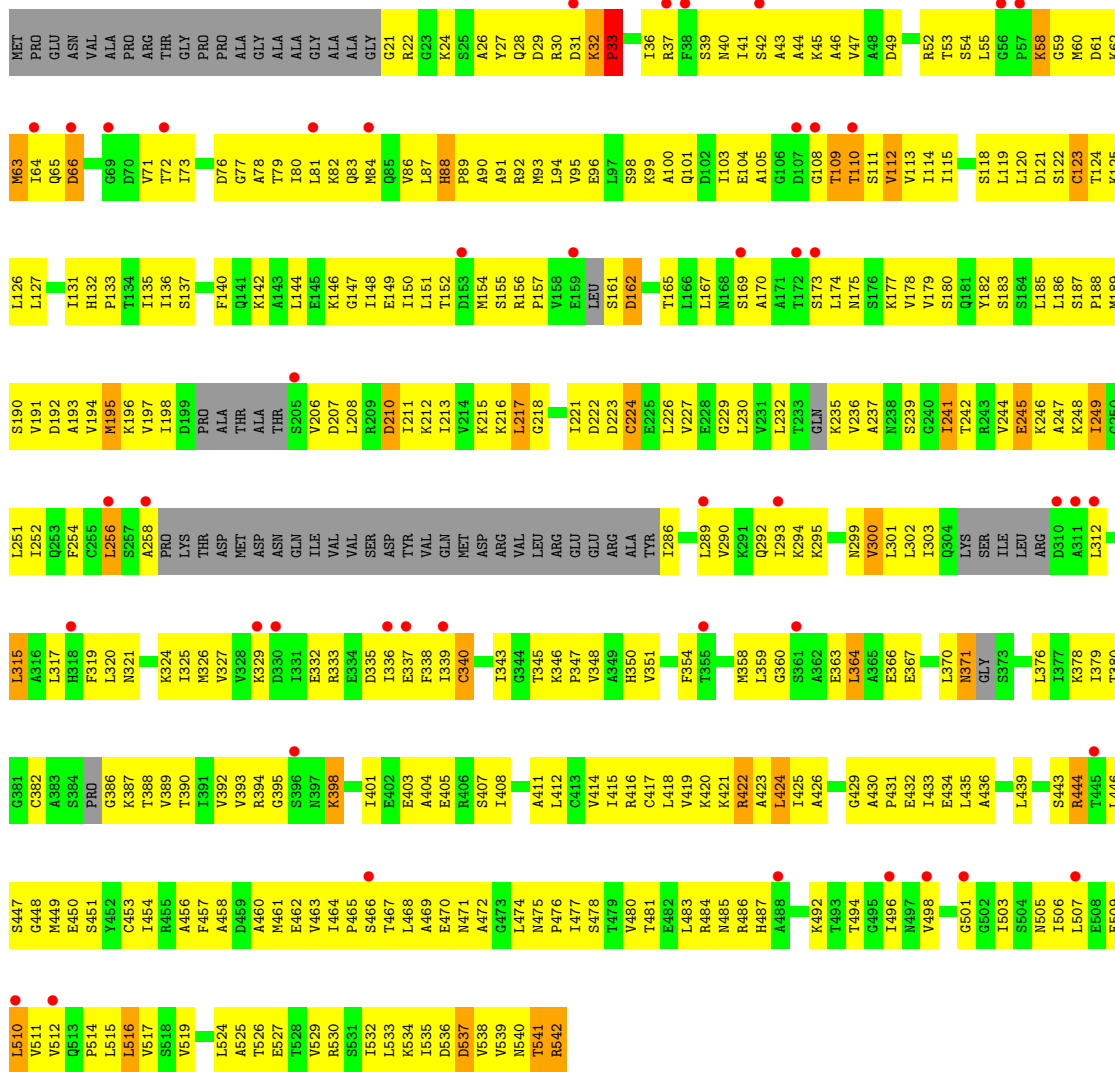
- Molecule 8 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ZETA.

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			



- Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA





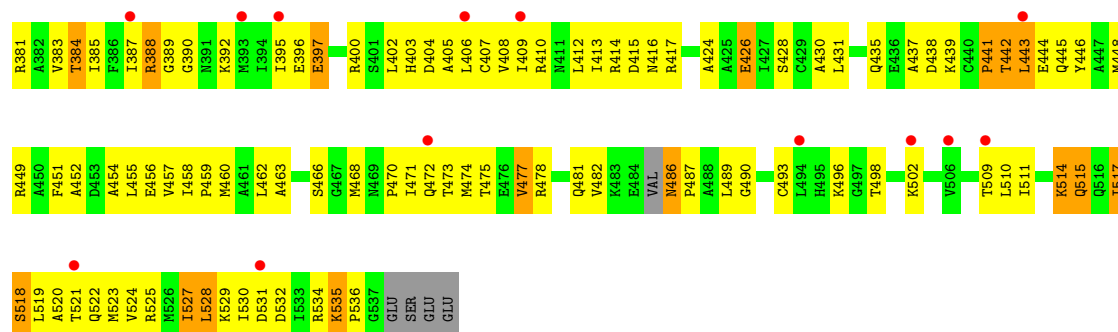
L1126	L1127	Q1128	K1129	G1130	I1131	H1132	P1133	I1136	S1137	S1138	F1140	L1144	E1145	G1146	G1147	I1148	E1149	I1150	L1151	T1152	L1153	M1154	S1155	P1156	P1157	V1158	E1159	L1160	S1161	D1162	R1163	E1164	T1165	L1166	L1167	N1168	S1169	A1170	T1171	S1172	S1173	L1174	N1175	S1176	K1177	V1178	V1179	S1180	Q1181	Y1182	L1185	L1186	S1187	P1188	M1189	S1190			
V1191	D1192	A1193	V1194	M1195	K1196	V1197	L1198	D1199	PRO	THR	ALA	THR	S1205	V1206	D1207	L1208	R1209	D1210	I1211	K1212	G1213	M1214	K1215	K1216	L1217	G1218	G1219	T1220	I1221	C1224	E1225	L1226	V1227	E1228	GLY	LEU	VAL	LEU	THR	GLN	LYS	VAL	ALA	ASN	SER	GLY	ILE	THR	THR	GLN	LYS	VAL	ALA	LYS	ILE	VAL	GLY	ASP	LEU
ILE	GLN	PHE	ASP	LEU	ALA	LEU	SER	ALA	HIS	PHE	LEU	LYS	PRO	THR	ASP	MET	LYS	ASP	ASN	GLN	ILE	VAL	VAL	ARG	GLU	ARG	GLY	ASP	ASP	ILE	ALA	ALA	HIS	VAL	LYS	VAL	GLN	ILE	THR	LYS	THR	ALA	ASP	NET	CYS	ASN	GLY	VAL	GLN	LYS	SER	GLU	VAL	ILE	GLY	ASP	ASN		
LEU	SER	ASP	LEU	ALA	LEU	SER	ALA	HIS	PHE	LEU	LYS	PRO	THR	ASP	MET	LYS	ASP	ILE	VAL	GLN	ILE	VAL	ARG	GLU	ARG	GLY	ASP	ASP	ILE	ALA	ALA	HIS	VAL	LYS	VAL	GLN	ILE	THR	LYS	THR	ALA	ASP	NET	CYS	ASN	GLY	VAL	GLN	LYS	SER	GLU	VAL	ILE	GLY	ASP	ASN			

N1497	V1498	R1499	G1500	G1501	L1502	I1503	S1504	N1505	L1506	L1507	E1508	E1509	L1510	V1511	Q1512	P1513	L1514	L1515	L1516	V1517	S1518	V1519	L1520	T1521	L1522	T1523	L1524	A1525	L1526	E1527	V1528	V1529	R1530	S1531	L1532	L1533	K1534	I1535	D1536	D1537	V1538	V1539	N1540	T1541	R1542															
E1434	L1435	A1436	L1437	L1438	L1439	T1440	E1441	R1444	T1445	L1446	S1447	G1448	M1449	E1450	S1451	L1452	C1453	L1454	R1455	A1456	F1457	L1458	D1459	A1460	M1461	E1462	V1463	L1464	P1465	S1466	T1467	A1468	A1469	E1470	N1471	A1472	G1473	L1474	P1475	N1476	I1477	S1478	T1479	V1480	T1481	E1482	L1483	R1484	L1485	R1486	H1487	A1488	K1489	A1490	T1491	L1492	E1493	T1494	G1495	I1496

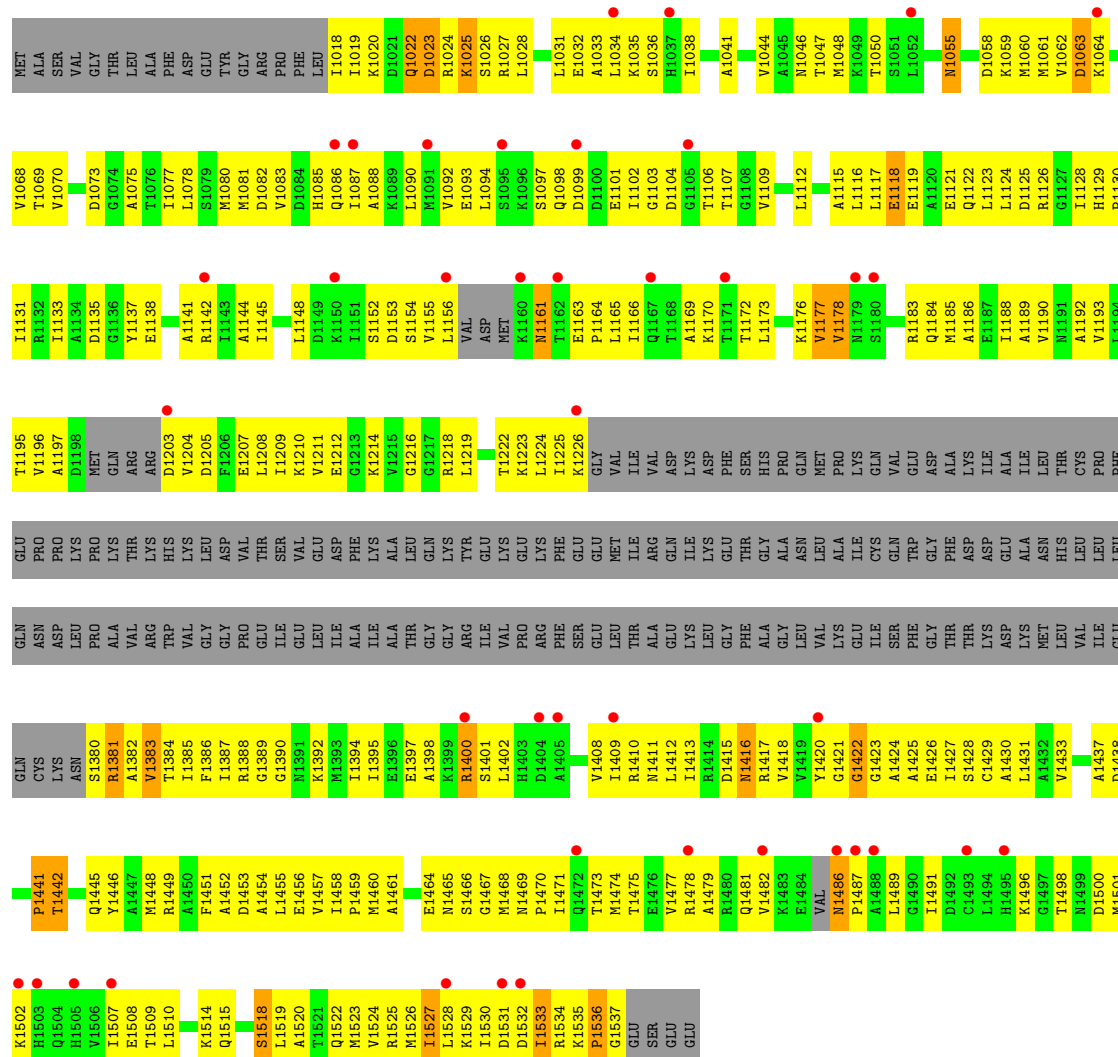
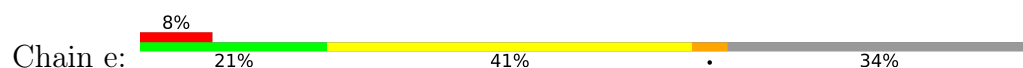
• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON



H312	L251	A189	Q122	V62	MET
L313	T252	A190	L123	D63	ALA
L314	C253	N191	L124	K64	SER
L315	P254	A192	D125	D65	VAL
Q316	E255	V193	R126	G66	GLY
N317	E256		G127	D67	THR
D318	P257	V196	I128	V68	LEU
L319	PRO	A197	H129	T69	ALA
P320	LYS	D198	P130	V70	PHE
A321	PRO	MET	I131	T71	ASP
V322	LYS	GLN	R132	M72	GLU
R323	THR	ARG	I133	D73	TYR
W324	LYS	ARG	A134	G74	GLY
V325	HIS	D203	D135	A75	ARG
E329	LYS	V204		T76	PRO
L330	LEU	D205	E138	I77	PHE
E331	ASP	F206	Q139	L78	LEU
L332	VAL	E207		S79	I18
L333	THR	L208	R142	M80	I19
T337	SER	I209	I143	M81	K20
R340	VAL	K210	A144	D82	D21
I341	GLU	V211	I145	V83	Q22
P343	ASP		E146	D84	D23
R344	PHE	K214	H147	H85	R24
F345	LYS	V215	L148	Q86	K25
S346	ALA	G216	D149	I87	S26
E347	LEU	G217	K150	A88	R27
L348	GLN	R218		K89	L28
E349	LYS	L219	D153	L90	M29
E351	TYR	E220	S154	M91	G30
K352	GLU	D221	L155	V92	L31
L353	LYS	T222	L156	E93	
K354	GLU	K223	VAL	L94	L34
L357	LYS	L224	ASP	S95	K35
G357	E285	I225	MET	K96	S36
K360	E286	K226	K160	S97	H37
E361		G227	N161	Q98	I38
L362	I289	V228	T162	D99	K39
S363	R290	I229	E163	D100	A40
F364	Q291	V230	E101	P164	A41
G365	L292	D231	L165	I102	K42
A366	K293	LYS	I166	G103	A43
THR	E294	ASP	Q167	D104	V44
K368	T295	F234	K170	G105	A45
D369	G296	S235	T171	T106	N46
K370	A297	H236	L172	G108	K48
K371	N298	P237	L173	V109	K49
L372	L299	Q238	G174	V110	T50
V373	A300	M239	S175	V111	S51
L374	I301	P240	K176	L112	L52
E375	C302	K241	S176	A113	G53
G376	Q303	Q242	V177	G114	P54
K377	W304	V243	V178	A115	N55
K378	G305	E244	R183	L116	G56
N379	F306	D245	Q184	L117	L57
S380	D307	A246	M185	E118	D58
	G308	K247	A186	E119	K59
	E309	I248	E187	A120	M60
	A310	A249	E187	E121	A61
	N311	I250	I189		

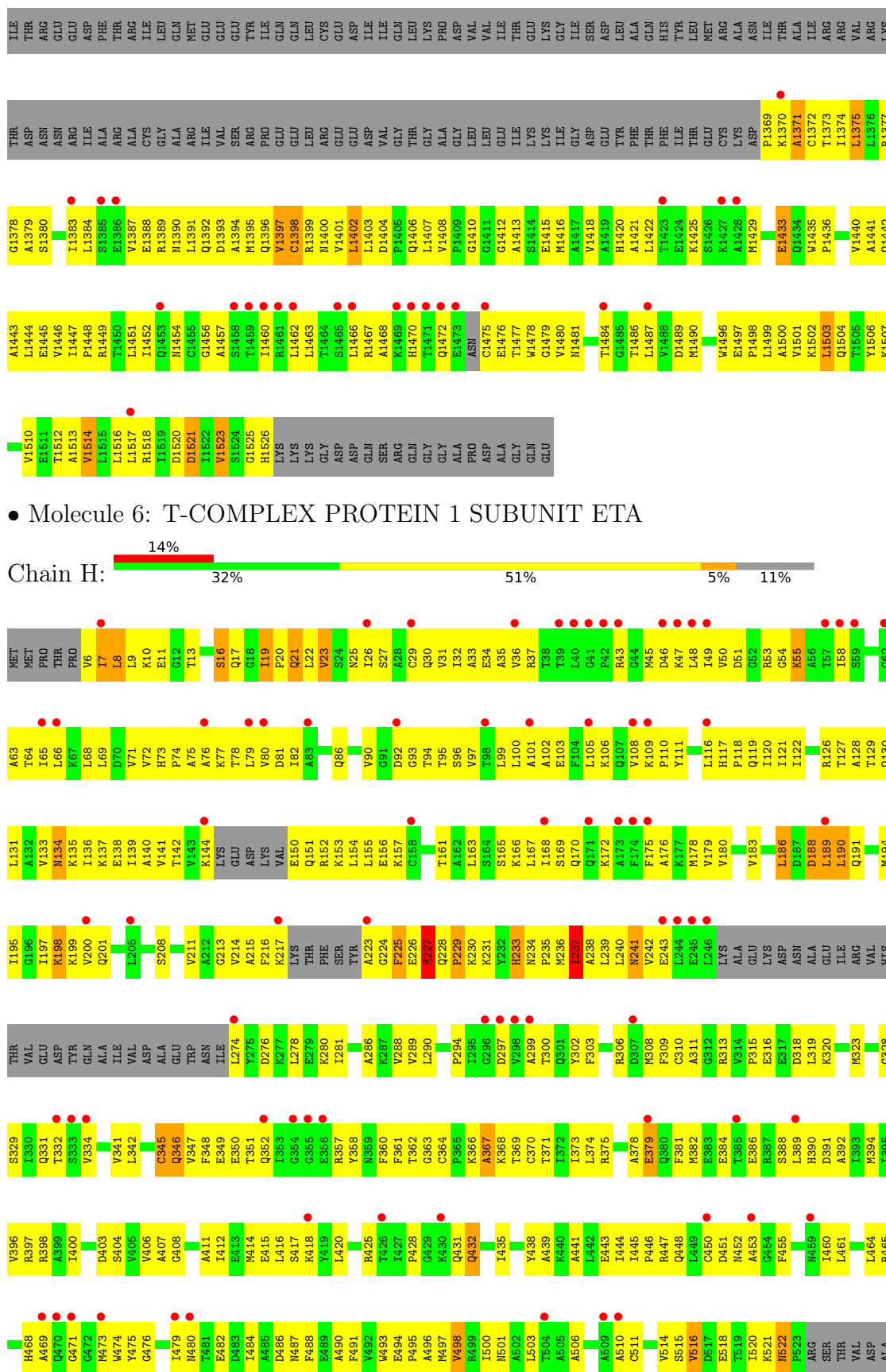


• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON



• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

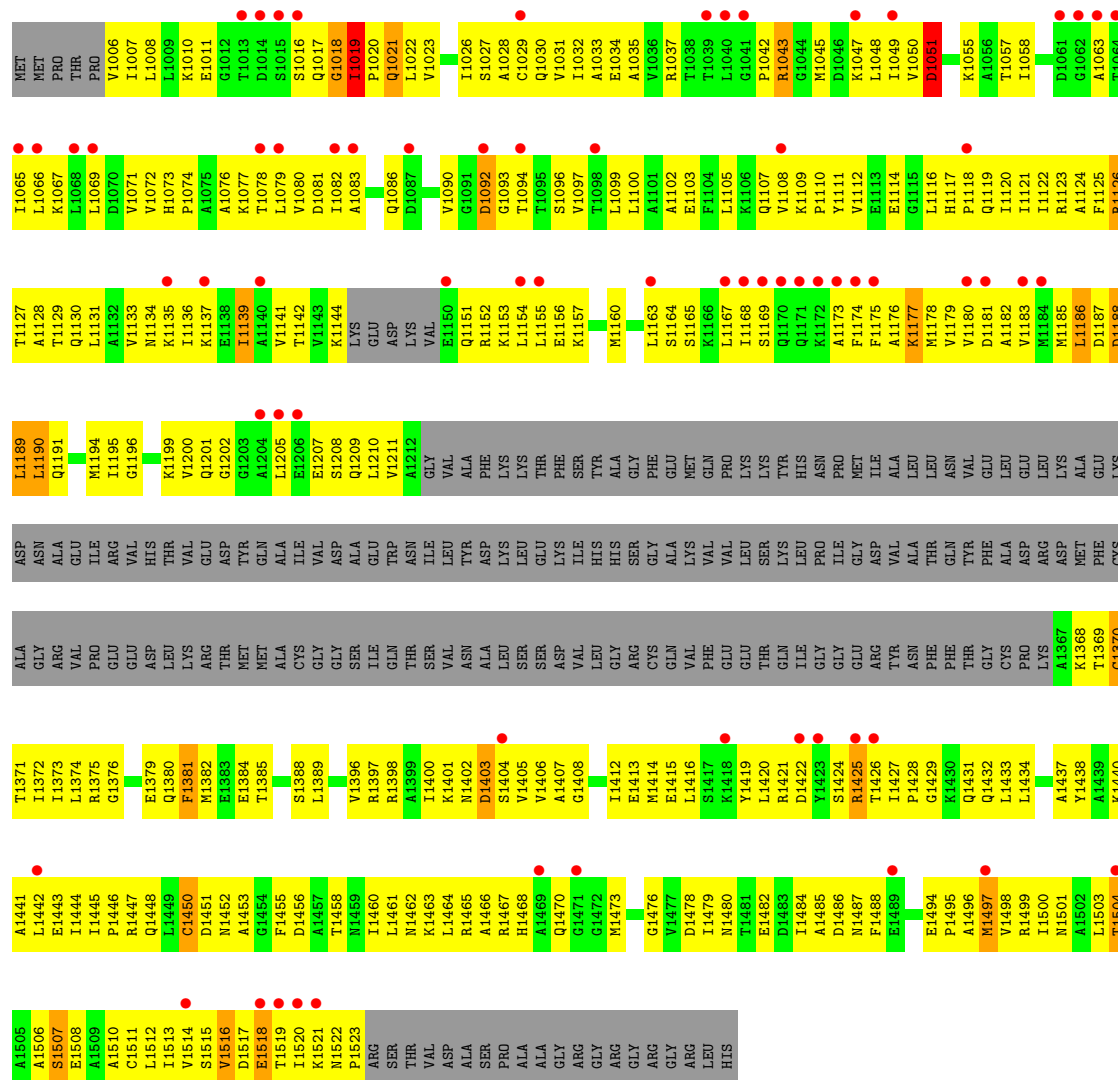




SER
PRO
ALA
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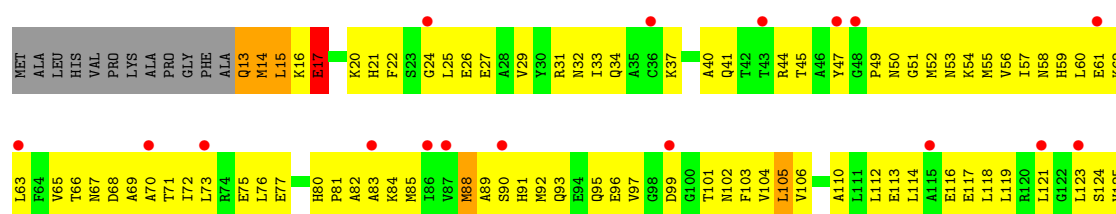
• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

Chain h: 13% 19% 43% 34%

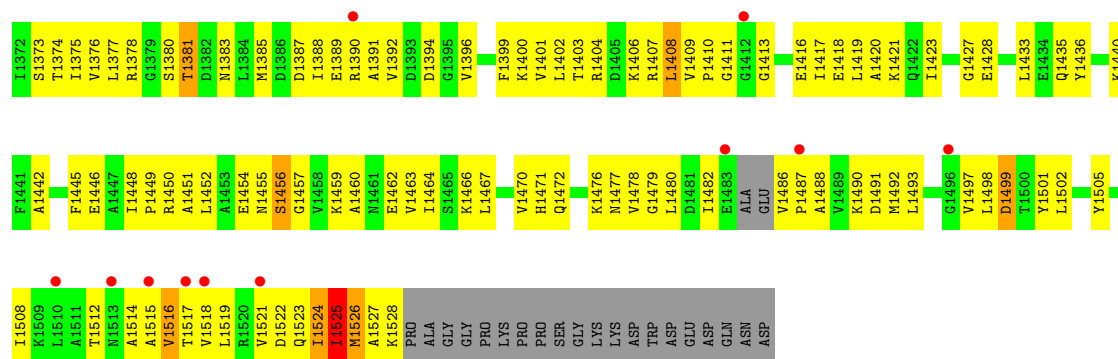


• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

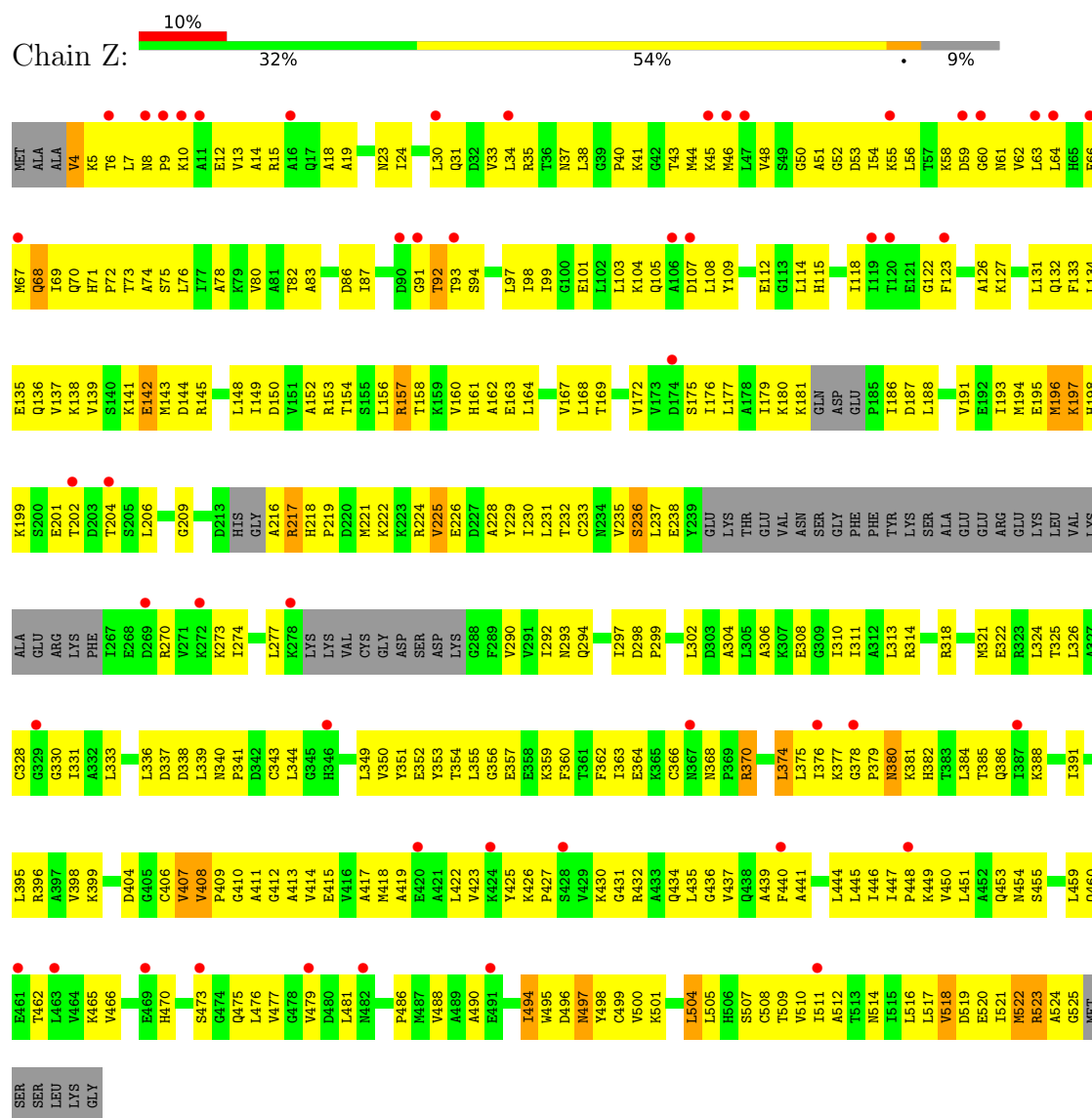
Chain Q: 13% 28% 55% 5% 12%







• 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	272.70Å 313.50Å 158.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 5.50 200.00 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (200.00-5.50) 99.1 (200.00-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 5.41Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.340 , 0.399 0.342 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	257.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 310.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/3657	0.74	0/4934
1	a	0.28	0/2733	0.76	0/3695
2	B	0.27	0/3638	0.75	1/4903 (0.0%)
2	b	0.27	0/2680	0.74	0/3615
3	D	0.27	0/3632	0.77	2/4891 (0.0%)
3	d	0.28	0/2707	0.77	0/3650
4	E	0.27	0/3712	0.75	0/4997
4	e	0.26	0/2743	0.74	0/3687
5	G	0.27	0/3758	0.76	3/5073 (0.1%)
5	g	0.27	0/2763	0.74	0/3733
6	H	0.27	0/3716	0.72	1/5008 (0.0%)
6	h	0.28	0/2751	0.76	2/3711 (0.1%)
7	Q	0.27	0/3724	0.74	1/5032 (0.0%)
7	q	0.26	0/2774	0.74	1/3746 (0.0%)
8	Z	0.26	0/3702	0.75	0/4995
8	z	0.27	0/3702	0.74	0/4995
All	All	0.27	0/52392	0.75	11/70665 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	h	1188	ASP	N-CA-C	-7.40	103.72	112.89
6	h	1019	ILE	CB-CA-C	-6.52	107.51	113.70
7	q	1525	ILE	N-CA-C	6.32	112.97	106.21
5	G	430	THR	CB-CA-C	-5.90	108.77	115.79
5	G	115	GLN	N-CA-C	-5.59	106.31	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3625	0	3783	409	0
1	a	2705	0	2799	465	0
2	B	3602	0	3705	376	0
2	b	2658	0	2733	296	0
3	D	3610	0	3810	481	0
3	d	2690	0	2818	364	0
4	E	3674	0	3781	413	0
4	e	2724	0	2822	328	0
5	G	3719	0	3870	416	0
5	g	2735	0	2851	316	0
6	H	3671	0	3783	389	0
6	h	2724	0	2842	343	0
7	Q	3673	0	3719	394	0
7	q	2739	0	2777	337	0
8	Z	3664	0	3820	432	0
8	z	3664	0	3820	426	0
All	All	51877	0	53733	5696	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 54.

The worst 5 of 5696 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1045:LEU:HD23	5:g:1523:VAL:HG11	1.12	1.12
1:a:1180:LYS:HG2	1:a:1403:LEU:HD21	1.23	1.10
1:a:1024:ALA:HA	5:g:1009:VAL:HG12	1.22	1.09
1:a:1173:VAL:HA	1:a:1399:VAL:HG21	1.36	1.07
6:H:425:ARG:HH21	1:a:1472:ASN:HB3	1.15	1.06

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/556 (85%)	390 (83%)	63 (13%)	18 (4%)	2	19
1	a	351/556 (63%)	283 (81%)	50 (14%)	18 (5%)	1	14
2	B	473/535 (88%)	398 (84%)	62 (13%)	13 (3%)	4	25
2	b	353/535 (66%)	301 (85%)	42 (12%)	10 (3%)	4	24
3	D	469/542 (86%)	385 (82%)	70 (15%)	14 (3%)	3	22
3	d	351/542 (65%)	300 (86%)	42 (12%)	9 (3%)	4	25
4	E	471/541 (87%)	392 (83%)	60 (13%)	19 (4%)	2	18
4	e	351/541 (65%)	295 (84%)	39 (11%)	17 (5%)	2	16
5	G	471/545 (86%)	396 (84%)	62 (13%)	13 (3%)	4	24
5	g	351/545 (64%)	291 (83%)	51 (14%)	9 (3%)	4	25
6	H	473/543 (87%)	384 (81%)	73 (15%)	16 (3%)	3	20
6	h	353/543 (65%)	289 (82%)	54 (15%)	10 (3%)	4	24
7	Q	473/548 (86%)	406 (86%)	45 (10%)	22 (5%)	2	16
7	q	351/548 (64%)	292 (83%)	48 (14%)	11 (3%)	3	21
8	Z	473/531 (89%)	400 (85%)	57 (12%)	16 (3%)	3	20
8	z	473/531 (89%)	403 (85%)	57 (12%)	13 (3%)	4	25
All	All	6708/8682 (77%)	5605 (84%)	875 (13%)	228 (3%)	3	20

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%)	363 (92%)	32 (8%)	11	31
1	a	297/461 (64%)	268 (90%)	29 (10%)	7	24
2	B	382/429 (89%)	370 (97%)	12 (3%)	35	56
2	b	281/429 (66%)	263 (94%)	18 (6%)	16	37
3	D	407/454 (90%)	386 (95%)	21 (5%)	21	42
3	d	303/454 (67%)	283 (93%)	20 (7%)	15	37
4	E	400/455 (88%)	374 (94%)	26 (6%)	15	37
4	e	298/455 (66%)	283 (95%)	15 (5%)	22	43
5	G	416/470 (88%)	399 (96%)	17 (4%)	27	48
5	g	307/470 (65%)	284 (92%)	23 (8%)	12	33
6	H	394/445 (88%)	377 (96%)	17 (4%)	26	47
6	h	292/445 (66%)	275 (94%)	17 (6%)	18	39
7	Q	398/452 (88%)	379 (95%)	19 (5%)	23	44
7	q	296/452 (66%)	280 (95%)	16 (5%)	20	41
8	Z	398/440 (90%)	383 (96%)	15 (4%)	29	50
8	z	398/440 (90%)	370 (93%)	28 (7%)	14	36
All	All	5662/7212 (78%)	5337 (94%)	325 (6%)	18	40

5 of 325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	e	1118	GLU
7	q	1173	TYR
4	e	1400	ARG
5	g	1402	LEU
8	z	1043	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	1464	GLN
6	h	1191	GLN
3	d	1141	GLN
4	e	1481	GLN
7	q	1013	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	481/556 (86%)	0.65	51 (10%) 11 17	260, 260, 260, 260	0
1	a	359/556 (64%)	1.03	73 (20%) 3 8	282, 282, 282, 282	0
2	B	481/535 (89%)	0.81	66 (13%) 6 14	281, 281, 281, 281	0
2	b	359/535 (67%)	0.72	50 (13%) 6 14	272, 272, 272, 272	0
3	D	481/542 (88%)	0.56	46 (9%) 13 20	289, 289, 289, 289	0
3	d	359/542 (66%)	0.93	66 (18%) 3 10	266, 266, 266, 266	0
4	E	481/541 (88%)	0.74	65 (13%) 7 14	262, 262, 262, 262	0
4	e	359/541 (66%)	0.60	41 (11%) 10 17	283, 283, 283, 283	0
5	G	481/545 (88%)	1.03	92 (19%) 3 9	283, 283, 283, 283	0
5	g	359/545 (65%)	0.81	55 (15%) 5 12	275, 275, 275, 275	0
6	H	481/543 (88%)	0.93	77 (16%) 5 11	272, 272, 272, 272	0
6	h	359/543 (66%)	0.91	68 (18%) 3 10	258, 258, 258, 258	0
7	Q	481/548 (87%)	0.85	71 (14%) 5 13	308, 308, 308, 308	0
7	q	359/548 (65%)	0.81	57 (15%) 5 11	261, 261, 261, 261	0
8	Z	481/531 (90%)	0.76	51 (10%) 11 17	297, 297, 297, 297	0
8	z	481/531 (90%)	1.15	98 (20%) 3 8	276, 276, 276, 276	0
All	All	6842/8682 (78%)	0.83	1027 (15%) 5 13	258, 276, 308, 308	0

The worst 5 of 1027 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	q	1073	LEU	11.5
8	z	1030	LEU	11.1
8	Z	63	LEU	10.3
6	H	243	GLU	9.7
6	h	1206	GLU	9.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.