wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 08:26 pm GMT

PDB ID	:	3ZQJ
Title	:	Mycobacterium tuberculosis UvrA
Authors	:	Rossi, F.; Khanduja, J.S.; Bortoluzzi, A.; Houghton, J.; Sander, P.; Guthlein, C.; Davis, E.O.; Springer, B.; Bottger, E.C.; Relini, A.; Penco, A.; Muniyappa, K.; Rizzi, M.
Deposited on	:	2011-06-09
Resolution	:	3.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

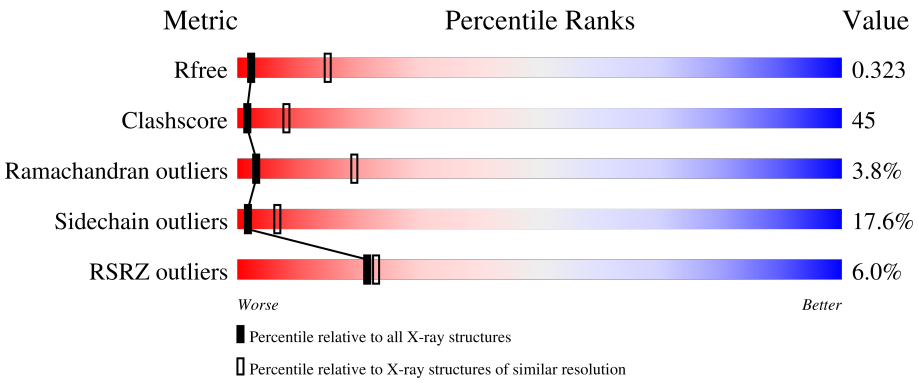
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	993	5%; 42%, 42%, 10%, • 5%
1	B	993	5%; 41%, 41%, 10%, • 8%
1	C	993	4%; 39%, 39%, 10%, • 10%
1	D	993	7%; 39%, 43%, 10%, • 7%
1	E	993	7%; 40%, 41%, 11%, • 7%

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Mol	Chain	Length	Quality of chain
1	F	993	5% 18% 32% 10% • 39%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 39998 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 UVRABC SYSTEM PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	944	7267	4550	1310	1385	22	0	0	0
1	B	918	7067	4428	1272	1345	22	0	0	0
1	C	890	6832	4277	1234	1299	22	0	0	0
1	D	921	7095	4444	1276	1353	22	0	0	0
1	E	919	7073	4434	1271	1347	21	0	0	0
1	F	607	4650	2906	844	890	10	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P63380
A	-19	GLY	-	expression tag	UNP P63380
A	-18	HIS	-	expression tag	UNP P63380
A	-17	HIS	-	expression tag	UNP P63380
A	-16	HIS	-	expression tag	UNP P63380
A	-15	HIS	-	expression tag	UNP P63380
A	-14	HIS	-	expression tag	UNP P63380
A	-13	HIS	-	expression tag	UNP P63380
A	-12	HIS	-	expression tag	UNP P63380
A	-11	HIS	-	expression tag	UNP P63380
A	-10	HIS	-	expression tag	UNP P63380
A	-9	HIS	-	expression tag	UNP P63380
A	-8	SER	-	expression tag	UNP P63380
A	-7	SER	-	expression tag	UNP P63380
A	-6	GLY	-	expression tag	UNP P63380
A	-5	HIS	-	expression tag	UNP P63380
A	-4	ILE	-	expression tag	UNP P63380

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP P63380
A	-2	GLY	-	expression tag	UNP P63380
A	-1	ARG	-	expression tag	UNP P63380
A	0	HIS	-	expression tag	UNP P63380
B	-20	MET	-	expression tag	UNP P63380
B	-19	GLY	-	expression tag	UNP P63380
B	-18	HIS	-	expression tag	UNP P63380
B	-17	HIS	-	expression tag	UNP P63380
B	-16	HIS	-	expression tag	UNP P63380
B	-15	HIS	-	expression tag	UNP P63380
B	-14	HIS	-	expression tag	UNP P63380
B	-13	HIS	-	expression tag	UNP P63380
B	-12	HIS	-	expression tag	UNP P63380
B	-11	HIS	-	expression tag	UNP P63380
B	-10	HIS	-	expression tag	UNP P63380
B	-9	HIS	-	expression tag	UNP P63380
B	-8	SER	-	expression tag	UNP P63380
B	-7	SER	-	expression tag	UNP P63380
B	-6	GLY	-	expression tag	UNP P63380
B	-5	HIS	-	expression tag	UNP P63380
B	-4	ILE	-	expression tag	UNP P63380
B	-3	GLU	-	expression tag	UNP P63380
B	-2	GLY	-	expression tag	UNP P63380
B	-1	ARG	-	expression tag	UNP P63380
B	0	HIS	-	expression tag	UNP P63380
C	-20	MET	-	expression tag	UNP P63380
C	-19	GLY	-	expression tag	UNP P63380
C	-18	HIS	-	expression tag	UNP P63380
C	-17	HIS	-	expression tag	UNP P63380
C	-16	HIS	-	expression tag	UNP P63380
C	-15	HIS	-	expression tag	UNP P63380
C	-14	HIS	-	expression tag	UNP P63380
C	-13	HIS	-	expression tag	UNP P63380
C	-12	HIS	-	expression tag	UNP P63380
C	-11	HIS	-	expression tag	UNP P63380
C	-10	HIS	-	expression tag	UNP P63380
C	-9	HIS	-	expression tag	UNP P63380
C	-8	SER	-	expression tag	UNP P63380
C	-7	SER	-	expression tag	UNP P63380
C	-6	GLY	-	expression tag	UNP P63380
C	-5	HIS	-	expression tag	UNP P63380
C	-4	ILE	-	expression tag	UNP P63380

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLU	-	expression tag	UNP P63380
C	-2	GLY	-	expression tag	UNP P63380
C	-1	ARG	-	expression tag	UNP P63380
C	0	HIS	-	expression tag	UNP P63380
D	-20	MET	-	expression tag	UNP P63380
D	-19	GLY	-	expression tag	UNP P63380
D	-18	HIS	-	expression tag	UNP P63380
D	-17	HIS	-	expression tag	UNP P63380
D	-16	HIS	-	expression tag	UNP P63380
D	-15	HIS	-	expression tag	UNP P63380
D	-14	HIS	-	expression tag	UNP P63380
D	-13	HIS	-	expression tag	UNP P63380
D	-12	HIS	-	expression tag	UNP P63380
D	-11	HIS	-	expression tag	UNP P63380
D	-10	HIS	-	expression tag	UNP P63380
D	-9	HIS	-	expression tag	UNP P63380
D	-8	SER	-	expression tag	UNP P63380
D	-7	SER	-	expression tag	UNP P63380
D	-6	GLY	-	expression tag	UNP P63380
D	-5	HIS	-	expression tag	UNP P63380
D	-4	ILE	-	expression tag	UNP P63380
D	-3	GLU	-	expression tag	UNP P63380
D	-2	GLY	-	expression tag	UNP P63380
D	-1	ARG	-	expression tag	UNP P63380
D	0	HIS	-	expression tag	UNP P63380
E	-20	MET	-	expression tag	UNP P63380
E	-19	GLY	-	expression tag	UNP P63380
E	-18	HIS	-	expression tag	UNP P63380
E	-17	HIS	-	expression tag	UNP P63380
E	-16	HIS	-	expression tag	UNP P63380
E	-15	HIS	-	expression tag	UNP P63380
E	-14	HIS	-	expression tag	UNP P63380
E	-13	HIS	-	expression tag	UNP P63380
E	-12	HIS	-	expression tag	UNP P63380
E	-11	HIS	-	expression tag	UNP P63380
E	-10	HIS	-	expression tag	UNP P63380
E	-9	HIS	-	expression tag	UNP P63380
E	-8	SER	-	expression tag	UNP P63380
E	-7	SER	-	expression tag	UNP P63380
E	-6	GLY	-	expression tag	UNP P63380
E	-5	HIS	-	expression tag	UNP P63380
E	-4	ILE	-	expression tag	UNP P63380

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLU	-	expression tag	UNP P63380
E	-2	GLY	-	expression tag	UNP P63380
E	-1	ARG	-	expression tag	UNP P63380
E	0	HIS	-	expression tag	UNP P63380
F	-20	MET	-	expression tag	UNP P63380
F	-19	GLY	-	expression tag	UNP P63380
F	-18	HIS	-	expression tag	UNP P63380
F	-17	HIS	-	expression tag	UNP P63380
F	-16	HIS	-	expression tag	UNP P63380
F	-15	HIS	-	expression tag	UNP P63380
F	-14	HIS	-	expression tag	UNP P63380
F	-13	HIS	-	expression tag	UNP P63380
F	-12	HIS	-	expression tag	UNP P63380
F	-11	HIS	-	expression tag	UNP P63380
F	-10	HIS	-	expression tag	UNP P63380
F	-9	HIS	-	expression tag	UNP P63380
F	-8	SER	-	expression tag	UNP P63380
F	-7	SER	-	expression tag	UNP P63380
F	-6	GLY	-	expression tag	UNP P63380
F	-5	HIS	-	expression tag	UNP P63380
F	-4	ILE	-	expression tag	UNP P63380
F	-3	GLU	-	expression tag	UNP P63380
F	-2	GLY	-	expression tag	UNP P63380
F	-1	ARG	-	expression tag	UNP P63380
F	0	HIS	-	expression tag	UNP P63380

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

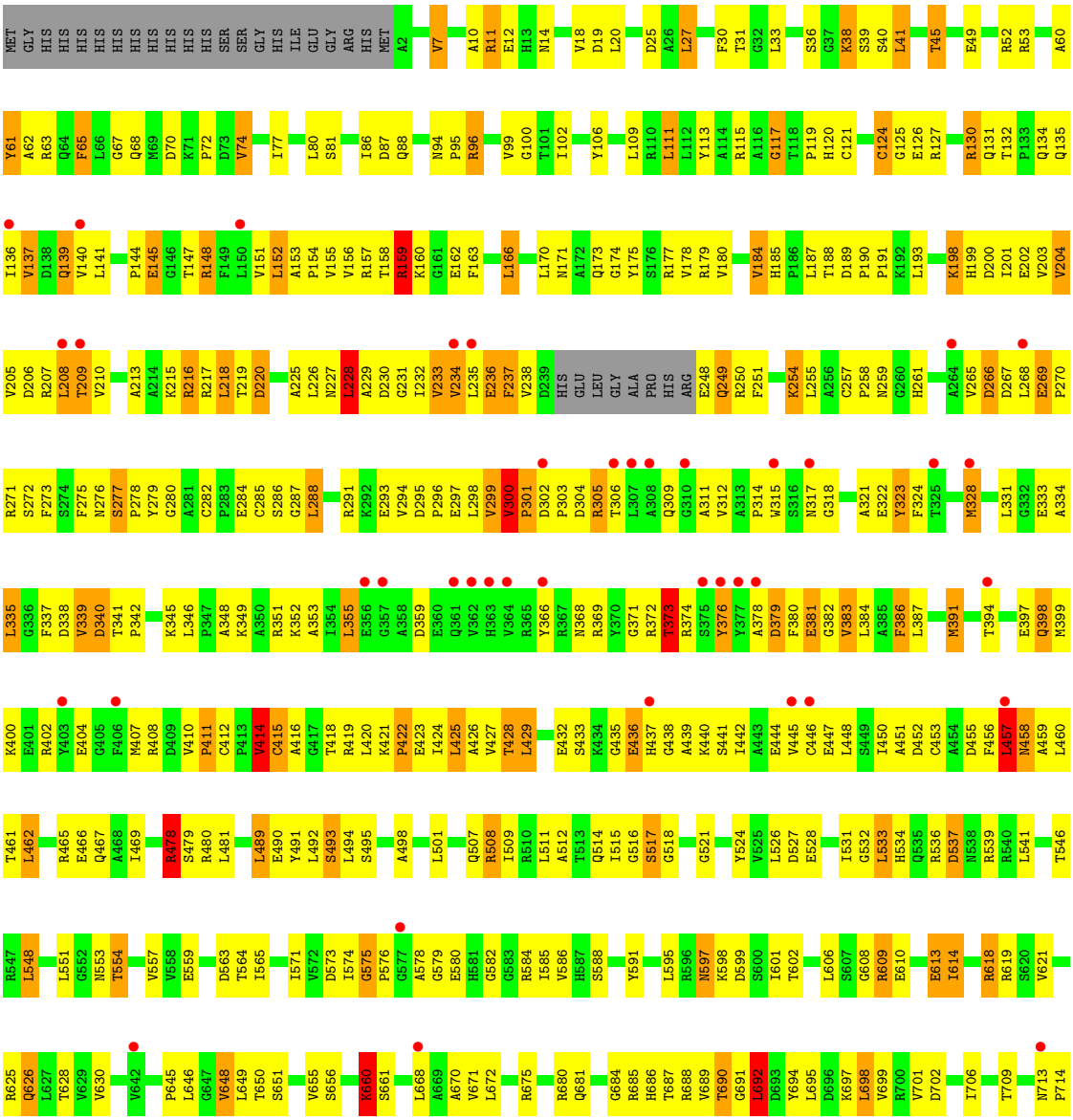
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	3	3	3	0	0
2	B	3	3	3	0	0
2	C	3	3	3	0	0
2	D	3	3	3	0	0
2	E	2	2	2	0	0

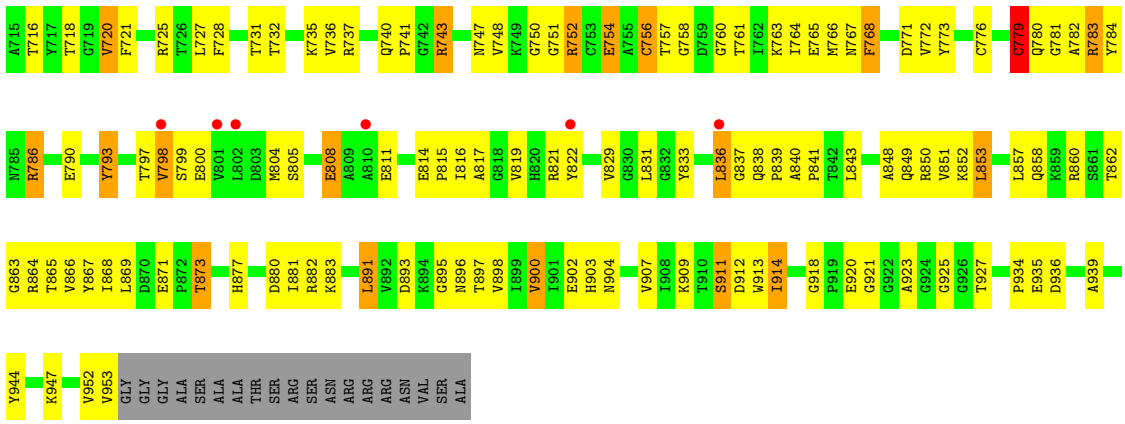
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: UVRABC SYSTEM PROTEIN A

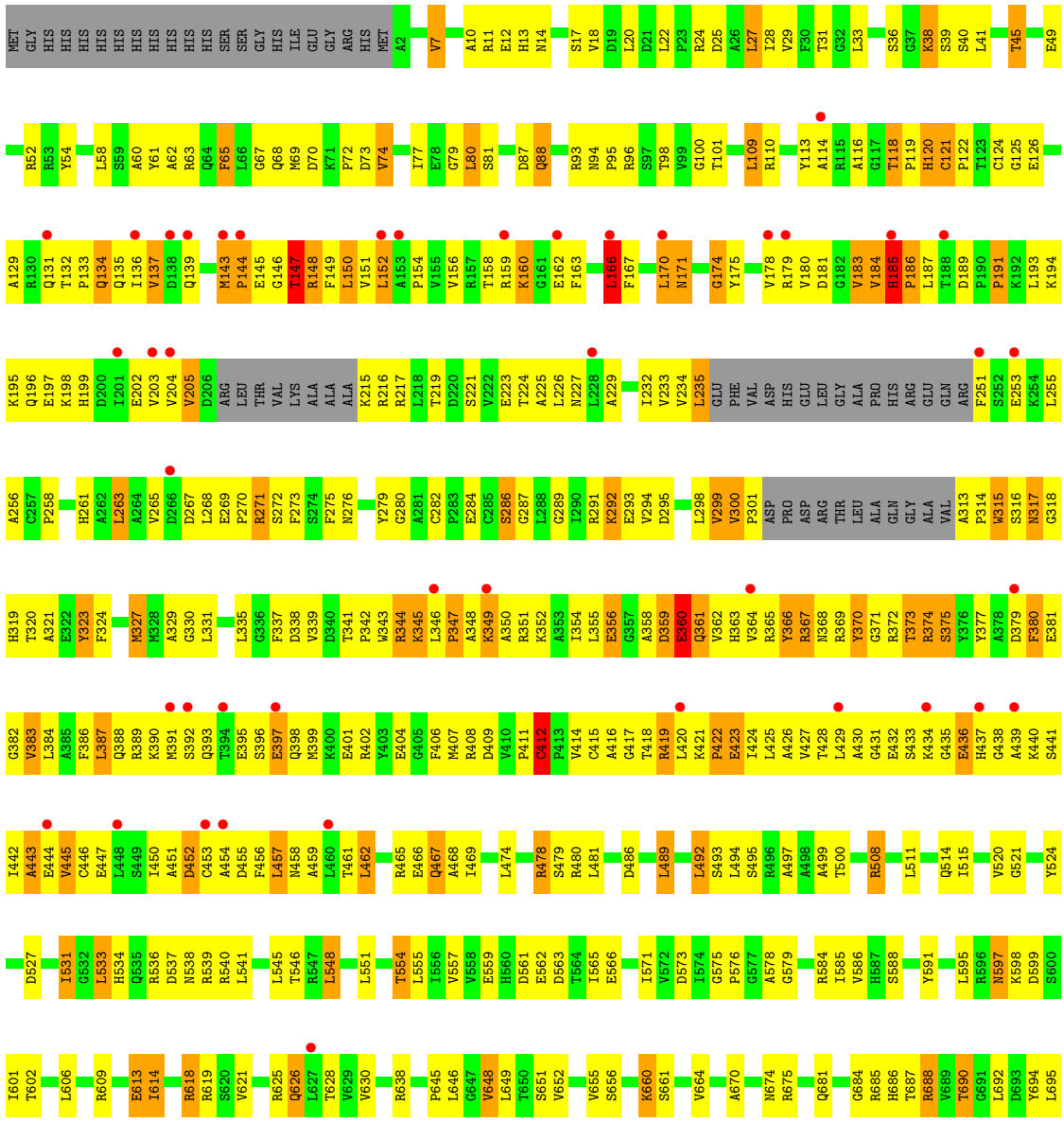
Chain A:

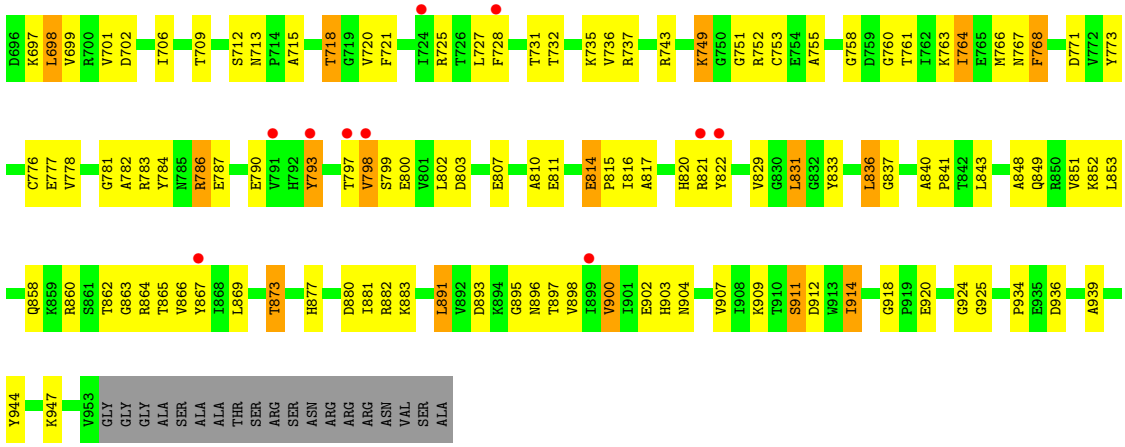




- Molecule 1: UVRABC SYSTEM PROTEIN A

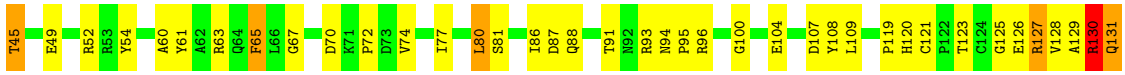
Chain B:

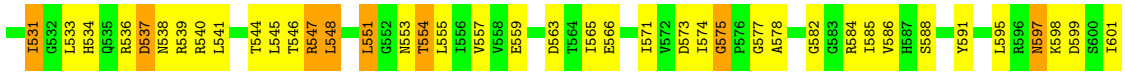


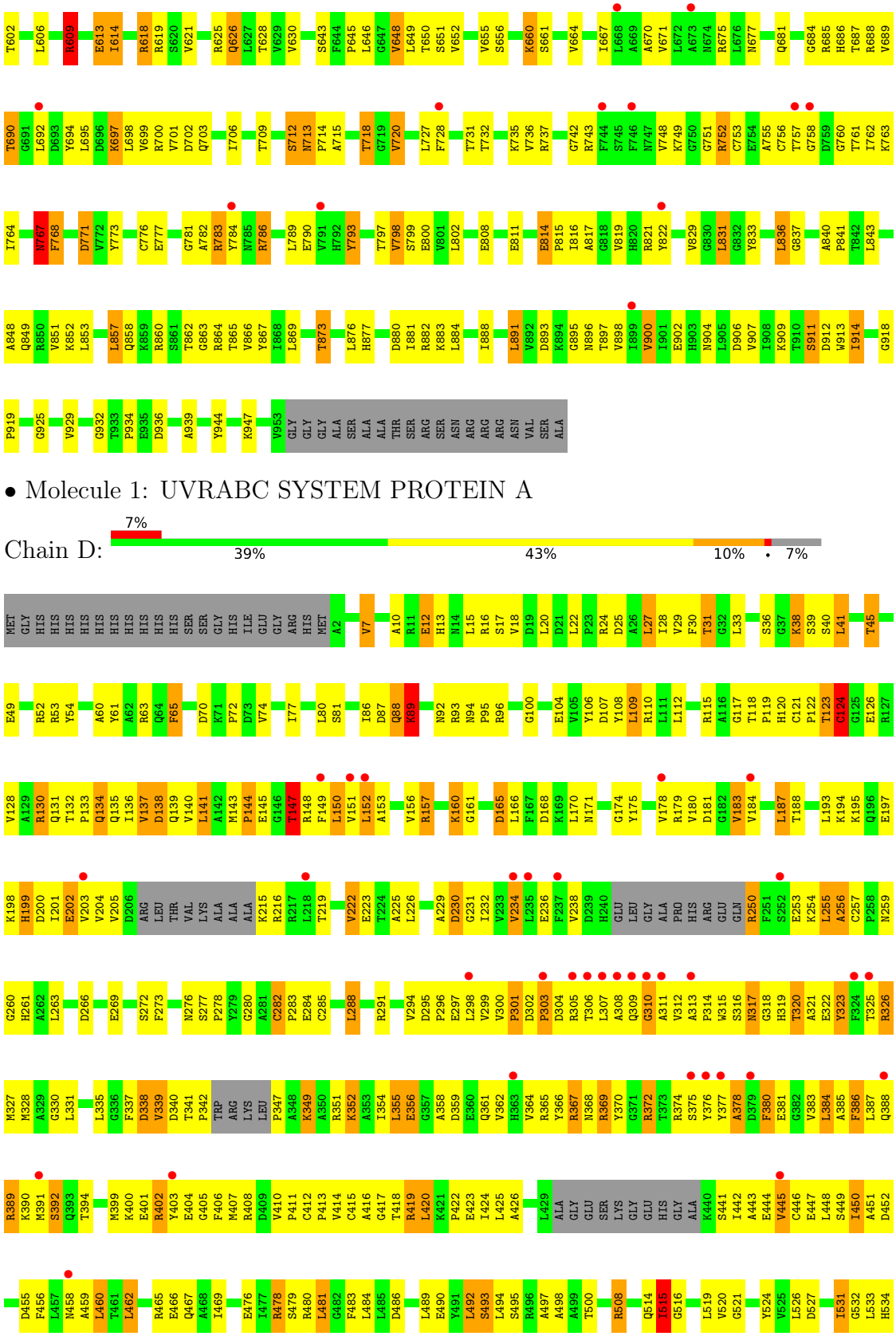


- Molecule 1: UVRABC SYSTEM PROTEIN A

Chain C:

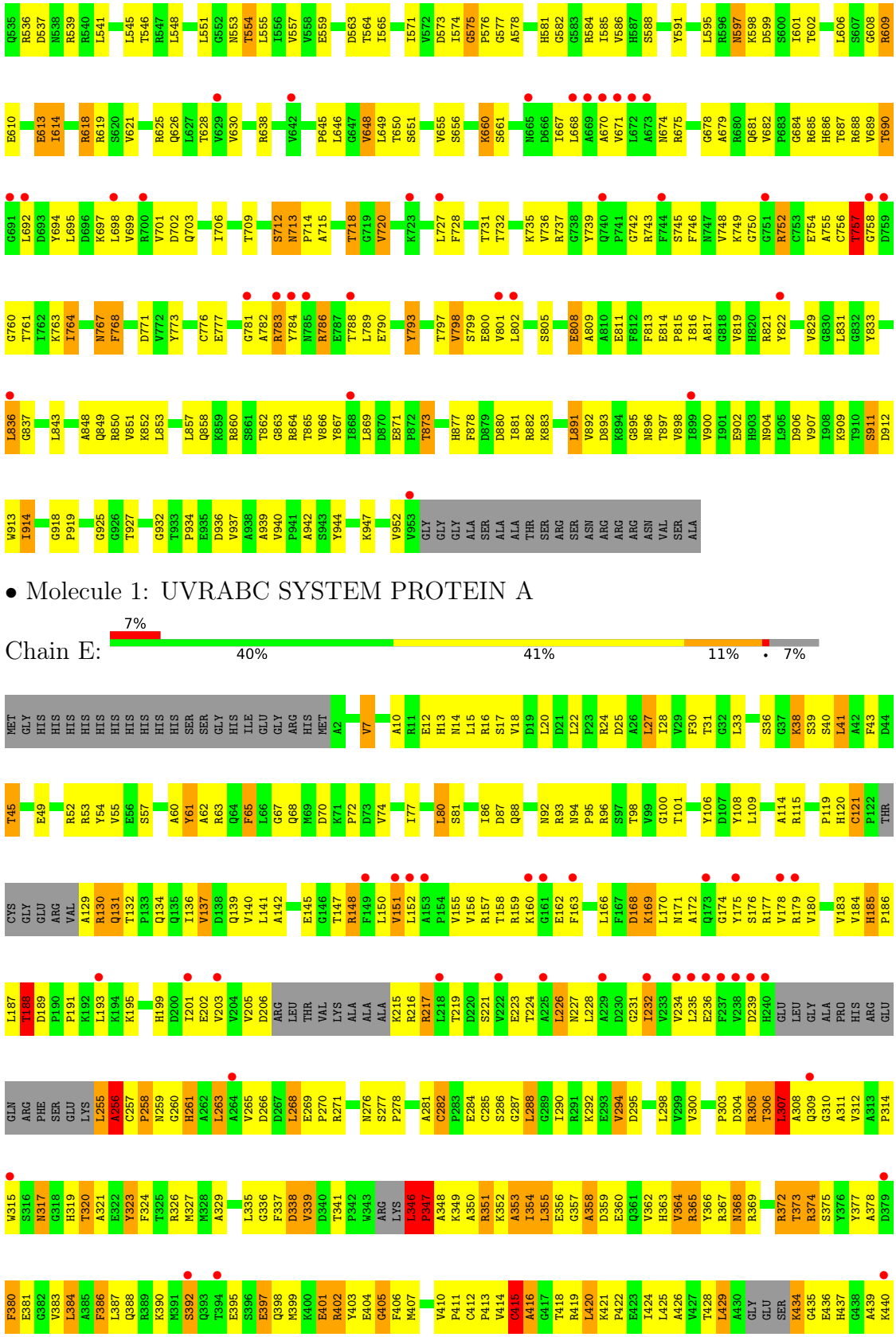






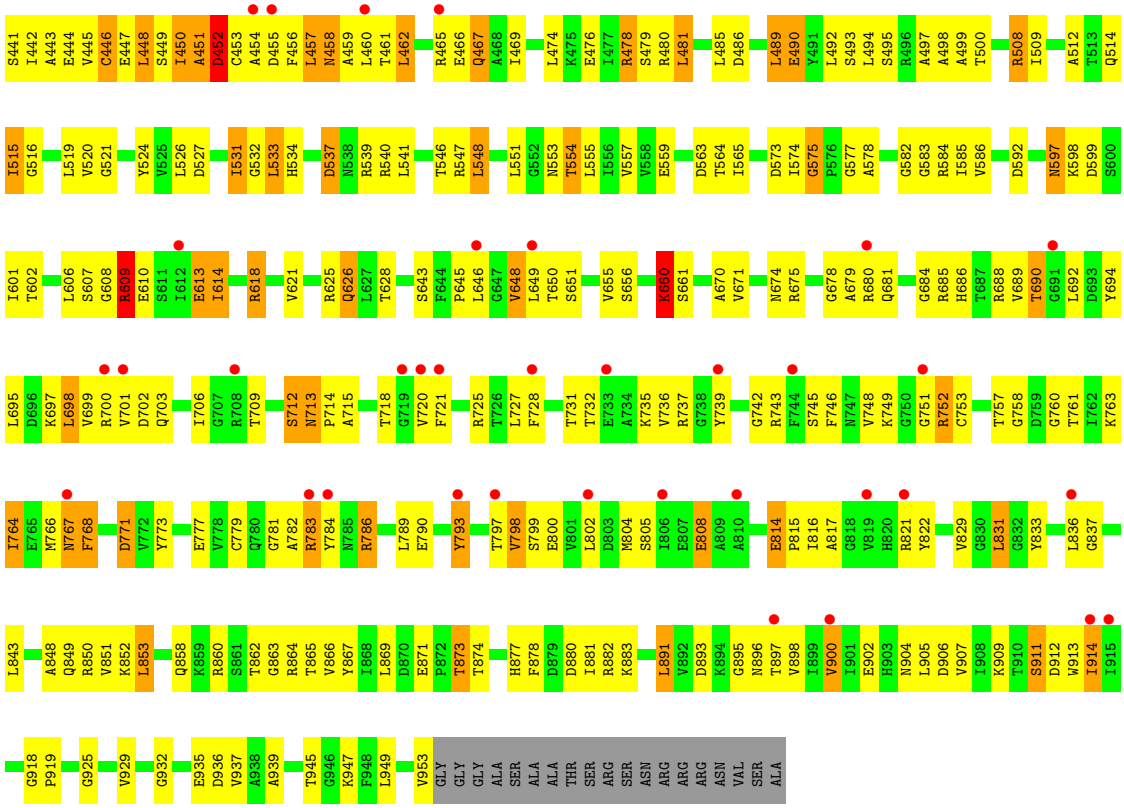
• Molecule 1: UVRABC SYSTEM PROTEIN A

Chain D: 7% 39% 43% 10% • 7%



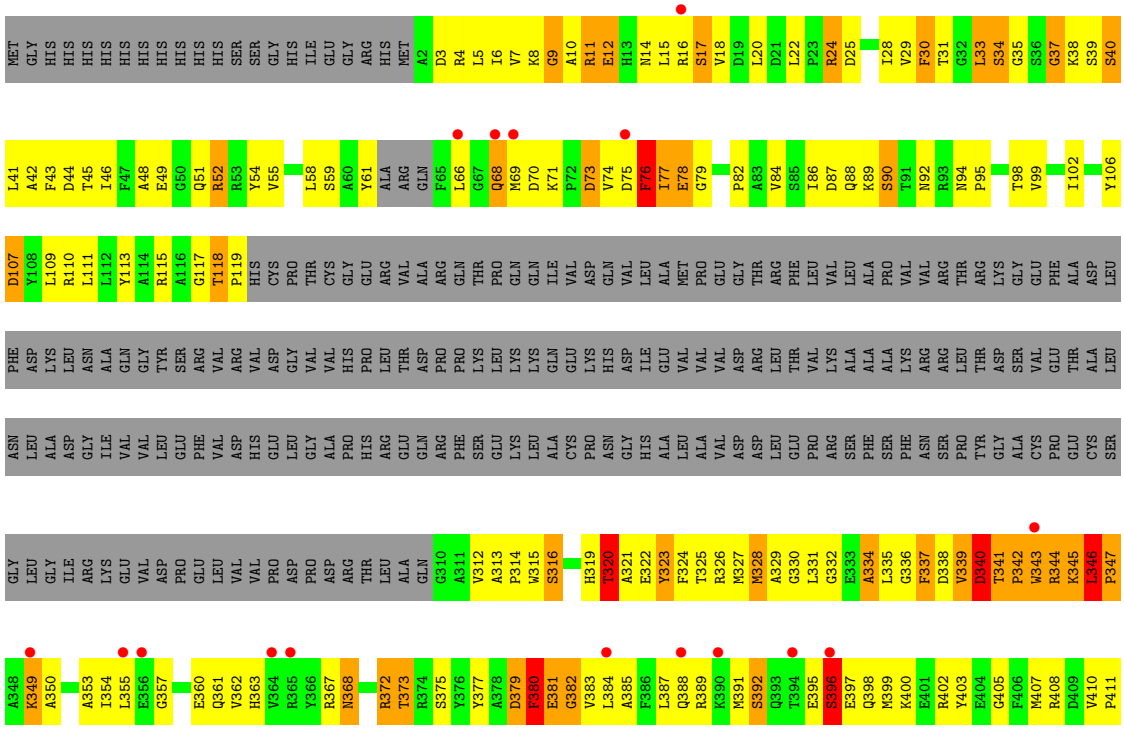
• Molecule 1: UVRABC SYSTEM PROTEIN A

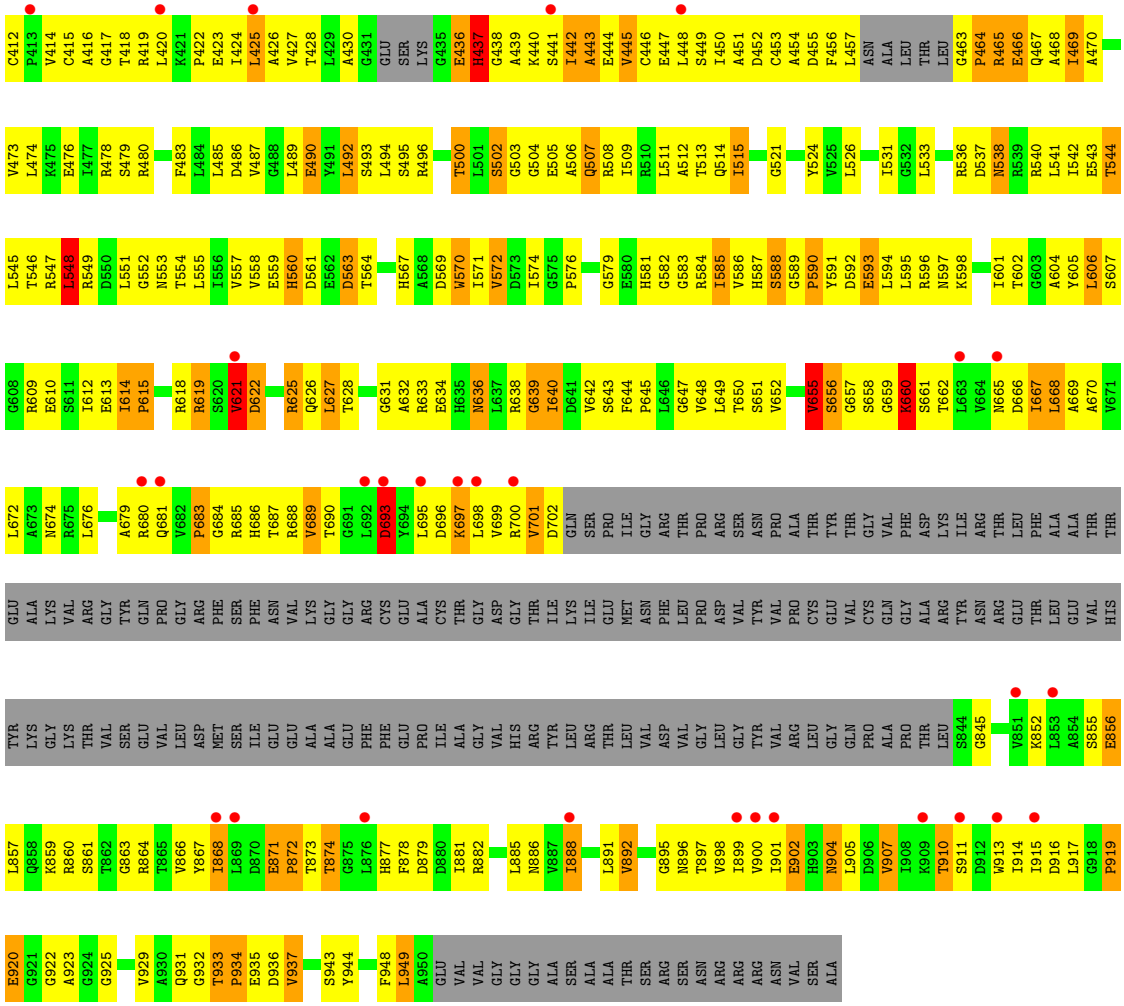
Chain E: 7% 40% 41% 11% • 7%



• Molecule 1: UVRABC SYSTEM PROTEIN A

Chain F: 5% 18% 32% 10% • 39%




C412 P413 V414 C415 A416 G417 T418 R419 L420 K421 P422 E423 I424 L425 A426 V427 T428 L429 A430 G431 GLU SER LYS G435 E436 H437 G438 A439 K440 S441 I442 A443 E444 V445 C446 E447 L448 S449 I450 A451 D452 C453 A454 D455 F456 L457 ASN ALA LEU THR LEU G463 P464 R465 E466 Q467 A468 I469 A470
V473 L474 K475 E476 I477 R478 S479 R480 F483 L484 L485 D486 V487 G488 L489 E490 Y491 L492 S493 L494 S495 R496 T500 L501 S502 G503 G504 E505 A506 Q507 R508 I509 R510 L511 A512 T513 Q514 I515 G521 Y524 V525 L526 I531 G532 L533 R536 D537 N538 R539 R540 L541 I542 E543 T544
L545 T546 R547 L548 R549 D550 L551 G552 N553 T554 L555 I556 V557 V558 E559 H560 D561 E562 D563 T564 H567 A568 D569 W570 I571 V572 D573 I574 G575 P576 G579 E580 H581 G582 G583 R584 I585 V586 H587 S588 G589 P590 Y591 D592 E593 L594 L595 R596 N597 K598 I601 T602 G603 A604 Y605 L606 S607
G608 R609 E610 S611 I612 E613 I614 P615 R618 R619 S620 V621 D622 R625 Q626 L627 T628 G631 A632 R633 E634 H635 N636 L637 R638 G639 I640 D641 V642 S643 F644 P645 L646 G647 V648 L649 T650 S651 V652 V655 S656 G657 S658 G659 K660 S661 T662 L663 V664 N665 D666 I667 L668 A669 A670 V671
L672 A673 N674 R675 L676 A679 R680 Q681 V682 P683 G684 R685 H686 T687 R688 V689 T690 G691 L692 D693 Y694 L695 D696 K697 L698 V699 R700 V701 D702 GLN SER PRO ILE GLY ARG THR PRO ARG SER ASN PRO ALA THR TYR THR GLY VAL PHE ASP LYS ILE ARG THR LEU PHE ALA ALA THR THR
GLU ALA LYS VAL ARG GLY TYR GLN PRO GLY ARG PHE SER PHE ASN VAL LYS GLY GLY ARG CYS GLU ALA CYS THR GLY ASP GLY THR ILE LYS ILE GLU MET ASN PHE LEU PRO ASP VAL TYR VAL PRO CYS GLU VAL CYS GLN GLY ALA ARG TYR ASN ARG GLU THR LEU GLU VAL HIS
TYR LYS GLY LYS THR VAL SER GLU VAL LEU ASP MET SER ILE GLU GLU ALA ALA GLU PHE PHE GLU PRO ILE ALA GLY VAL HIS ARG TYR LEU ARG THR LEU VAL ASP VAL GLY LEU GLY TYR VAL ARG LEU GLY GLN PRO ALA PRO THR LEU S844 G845 V851 K852 L853 A854 S855 E856
L857 Q858 K859 R860 S861 T862 G863 R864 T865 V866 Y867 I868 L869 D870 E871 P872 T873 T874 G875 L876 H877 F878 D879 D880 I881 R882 L885 N886 V887 I888 L891 V892 G895 N896 T897 V898 I899 V900 I901 E902 H903 N904 L905 D906 V907 I908 K909 T910 S911 D912 W913 I914 I915 D916 L917 G918 P919
E920 G921 G922 A923 G924 G925 V929 A930 Q931 G932 T933 P934 E935 D936 V937 S943 Y944 F948 L949 A950 GLU VAL VAL GLY GLY GLY ALA SER ALA ALA THR SER ARG SER ASN ARG ARG ARG ASN VAL SER ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	258.23Å 258.23Å 204.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.40 84.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.40) 98.5 (84.52-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.273 , 0.324 0.268 , 0.323	Depositor DCC
R_{free} test set	1067 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	83.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 69.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	39998	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.72	5/7394 (0.1%)	0.95	28/10021 (0.3%)
1	B	0.71	3/7190 (0.0%)	0.87	20/9741 (0.2%)
1	C	0.70	2/6945 (0.0%)	0.87	17/9406 (0.2%)
1	D	0.77	6/7217 (0.1%)	0.87	12/9779 (0.1%)
1	E	0.73	2/7196 (0.0%)	0.91	19/9753 (0.2%)
1	F	0.68	2/4721 (0.0%)	0.92	11/6385 (0.2%)
All	All	0.72	20/40663 (0.0%)	0.90	107/55085 (0.2%)

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
1	A	0	6
1	B	0	1
1	C	0	6
1	D	0	4
1	E	0	4
1	F	0	6
All	All	0	27

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	256	ALA	C-N	-13.62	1.02	1.34
1	D	124	CYS	C-N	12.92	1.56	1.33
1	D	126	GLU	C-N	-11.61	1.07	1.34
1	B	120	HIS	C-N	-11.33	1.07	1.34
1	A	415	CYS	C-N	11.23	1.59	1.34

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	478	ARG	NE-CZ-NH1	17.05	128.83	120.30
1	A	478	ARG	NE-CZ-NH2	-16.13	112.23	120.30
1	A	752	ARG	NE-CZ-NH2	-14.18	113.21	120.30
1	A	752	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	E	307	LEU	CB-CA-C	-12.39	86.66	110.20

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Mainchain
1	A	148	ARG	Sidechain
1	A	213	ALA	Peptide
1	A	373	THR	Peptide
1	A	411	PRO	Mainchain

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	7267	0	7280	633	1
1	B	7067	0	7080	707	3
1	C	6832	0	6855	556	0
1	D	7095	0	7100	590	0
1	E	7073	0	7081	602	4
1	F	4650	0	4667	567	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
All	All	39998	0	40063	3590	5

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 45.

The worst 5 of 3590 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:E:442:ILE:HA	1:E:495:SER:CB	1.23	1.62
1:B:299:VAL:HG23	1:B:313:ALA:CB	1.23	1.58
1:D:305:ARG:HA	1:D:311:ALA:CB	1.28	1.57
1:B:299:VAL:CG2	1:B:313:ALA:HB2	1.29	1.56
1:F:412:CYS:SG	1:F:414:VAL:HG22	1.47	1.52

All (5) 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)
1:E:597:ASN:OD1	1:F:16:ARG:NH1[4_554]	2.07	0.13
1:B:398:GLN:OE1	1:E:366:TYR:CB[6_444]	2.09	0.11
1:B:398:GLN:OE1	1:E:366:TYR:CD2[6_444]	2.09	0.11
1:B:398:GLN:OE1	1:E:366:TYR:CG[6_444]	2.09	0.11
1:A:61:TYR:CE2	1:A:767:ASN:O[4_555]	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	A	940/993 (95%)	814 (87%)	105 (11%)	21 (2%)	6 29
1	B	910/993 (92%)	768 (84%)	112 (12%)	30 (3%)	4 22
1	C	876/993 (88%)	730 (83%)	109 (12%)	37 (4%)	3 18
1	D	911/993 (92%)	758 (83%)	123 (14%)	30 (3%)	4 22
1	E	907/993 (91%)	750 (83%)	128 (14%)	29 (3%)	4 22
1	F	595/993 (60%)	449 (76%)	98 (16%)	48 (8%)	1 5
All	All	5139/5958 (86%)	4269 (83%)	675 (13%)	195 (4%)	3 19

5 of 195 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	VAL
1	A	300	VAL
1	A	301	PRO
1	A	382	GLY
1	A	457	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	778/815 (96%)	648 (83%)	130 (17%)	2 8
1	B	758/815 (93%)	640 (84%)	118 (16%)	2 11
1	C	732/815 (90%)	594 (81%)	138 (19%)	1 4
1	D	763/815 (94%)	642 (84%)	121 (16%)	2 10
1	E	758/815 (93%)	616 (81%)	142 (19%)	1 5
1	F	492/815 (60%)	386 (78%)	106 (22%)	1 3
All	All	4281/4890 (88%)	3526 (82%)	755 (18%)	2 6

5 of 755 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	546	THR
1	E	398	GLN
1	D	660	LYS
1	D	541	LEU
1	E	121	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	317	ASN
1	E	88	GLN
1	D	538	ASN
1	D	767	ASN

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Mol	Chain	Res	Type
1	E	398	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	A	2
1	B	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	260:GLY	C	261:HIS	N	1.19
1	A	11:ARG	C	12:GLU	N	1.15
1	A	411:PRO	C	412:CYS	N	1.11
1	B	120:HIS	C	121:CYS	N	1.08
1	D	126:GLU	C	127:ARG	N	1.07

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	944/993 (95%)	0.47	46 (4%)	29	29	16, 55, 94, 112	0
1	B	918/993 (92%)	0.44	53 (5%)	23	24	16, 57, 102, 111	0
1	C	890/993 (89%)	0.37	35 (3%)	39	38	16, 60, 108, 118	0
1	D	921/993 (92%)	0.43	65 (7%)	16	18	16, 60, 103, 114	0
1	E	919/993 (92%)	0.46	68 (7%)	14	16	16, 57, 102, 127	0
1	F	607/993 (61%)	0.53	45 (7%)	14	16	45, 79, 112, 117	0
All	All	5199/5958 (87%)	0.44	312 (6%)	21	23	16, 61, 104, 127	0

The worst 5 of 312 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	GLY	7.0
1	E	239	ASP	6.8
1	D	235	LEU	6.7
1	A	308	ALA	6.5
1	A	307	LEU	6.1

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	ZN	A	1954	1/1	0.75	0.20	65,65,65,65	0
2	ZN	B	1955	1/1	0.80	0.26	116,116,116,116	0
2	ZN	A	1955	1/1	0.83	0.21	116,116,116,116	0
2	ZN	E	1955	1/1	0.85	0.24	116,116,116,116	0
2	ZN	D	1955	1/1	0.89	0.23	116,116,116,116	0
2	ZN	C	1955	1/1	0.93	0.23	116,116,116,116	0
2	ZN	A	1956	1/1	0.94	0.21	48,48,48,48	0
2	ZN	B	1956	1/1	0.95	0.19	44,44,44,44	0
2	ZN	B	1954	1/1	0.95	0.21	65,65,65,65	0
2	ZN	D	1954	1/1	0.96	0.13	66,66,66,66	0
2	ZN	E	1954	1/1	0.98	0.17	66,66,66,66	0
2	ZN	D	1956	1/1	0.99	0.16	59,59,59,59	0
2	ZN	C	1954	1/1	0.99	0.17	65,65,65,65	0
2	ZN	C	1956	1/1	0.99	0.18	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.