



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:33 PM UTC

PDB ID : 2IPC / pdb_00002ipc
Title : Crystal structure of the translocation ATPase SecA from *Thermus thermophilus* reveals a parallel, head-to-head dimer
Authors : Vassylyev, D.G.; Mori, H.; Vassylyeva, M.N.; Tsukazaki, T.; Kimura, Y.; Tahirov, T.H.; Ito, K.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-10-12
Resolution : 2.80 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

<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
Xtrriage (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

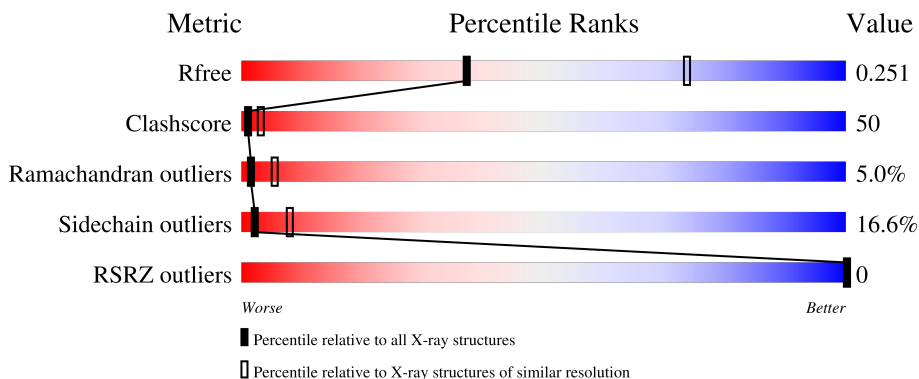
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	997	 28% 50% 14% • 6%
1	B	997	 29% 47% 14% • 6%
1	C	997	 28% 50% 14% • 6%
1	D	997	 27% 50% 14% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31502 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 Preprotein translocase SecA subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	939	7551	4774	1354	1399	24	0	0	0
1	B	934	7515	4749	1349	1394	23	0	0	0
1	C	939	7551	4774	1354	1399	24	0	0	0
1	D	934	7515	4749	1349	1394	23	0	0	0

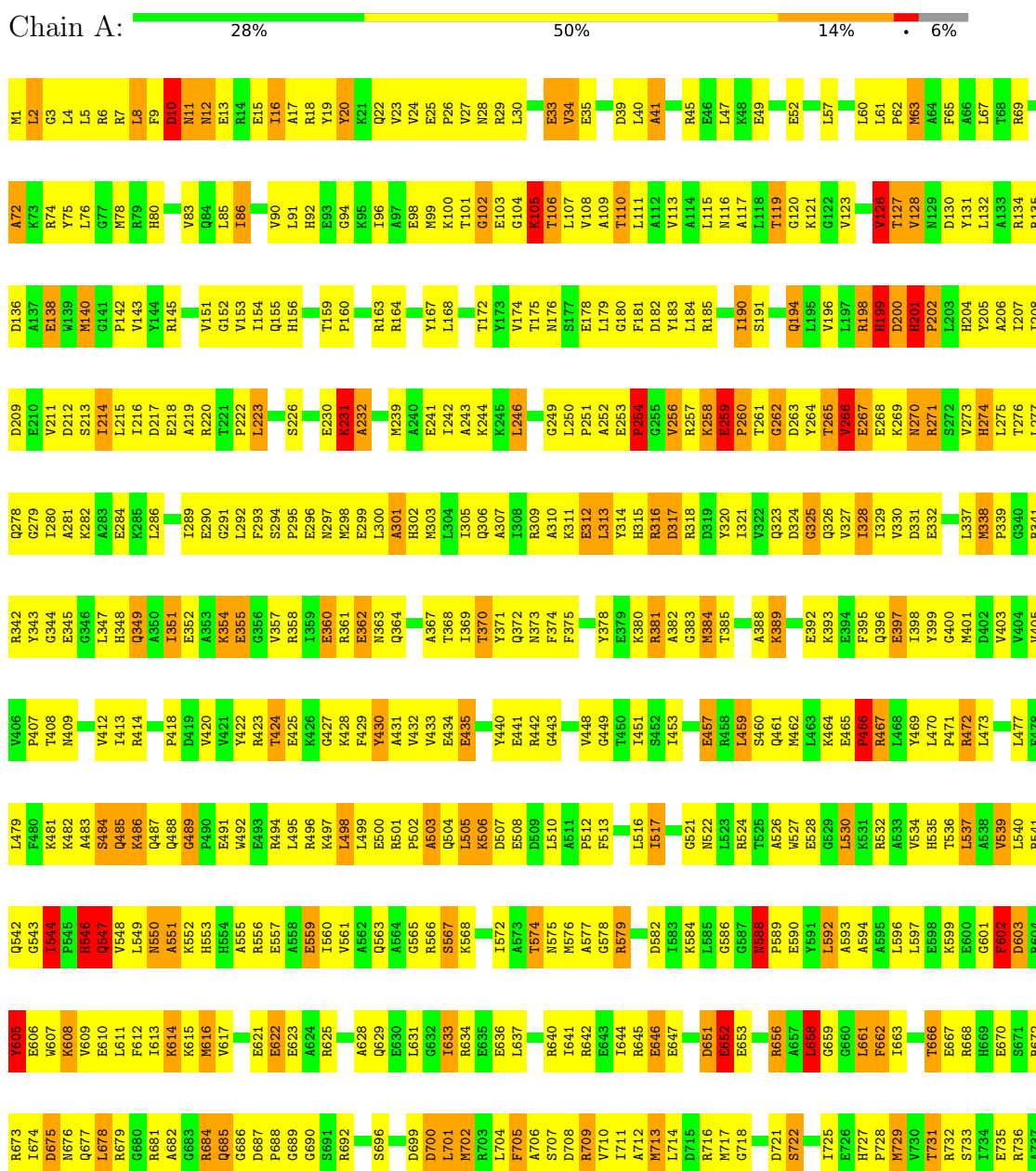
- Molecule 2 is water.

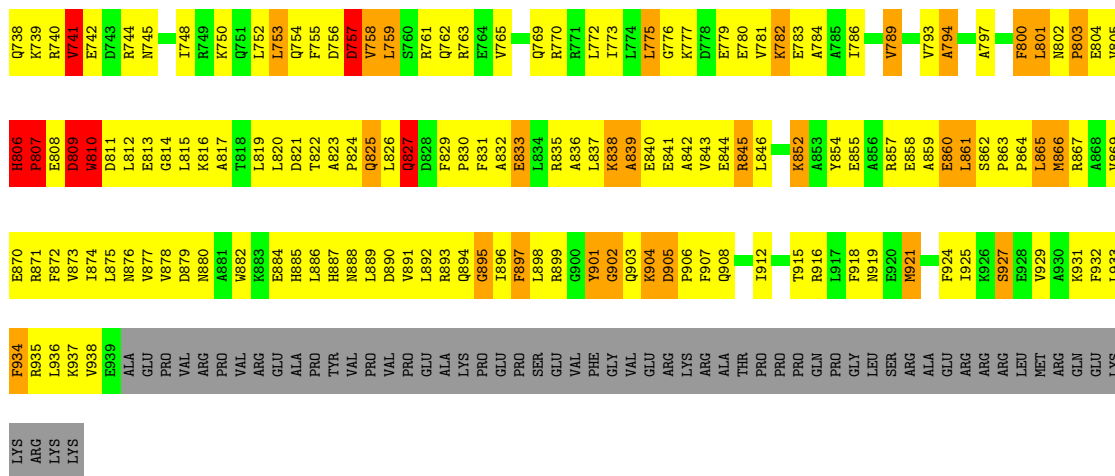
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	359	Total	O	0	0
			359	359		
2	B	320	Total	O	0	0
			320	320		
2	C	344	Total	O	0	0
			344	344		
2	D	347	Total	O	0	0
			347	347		

3 Residue-property plots

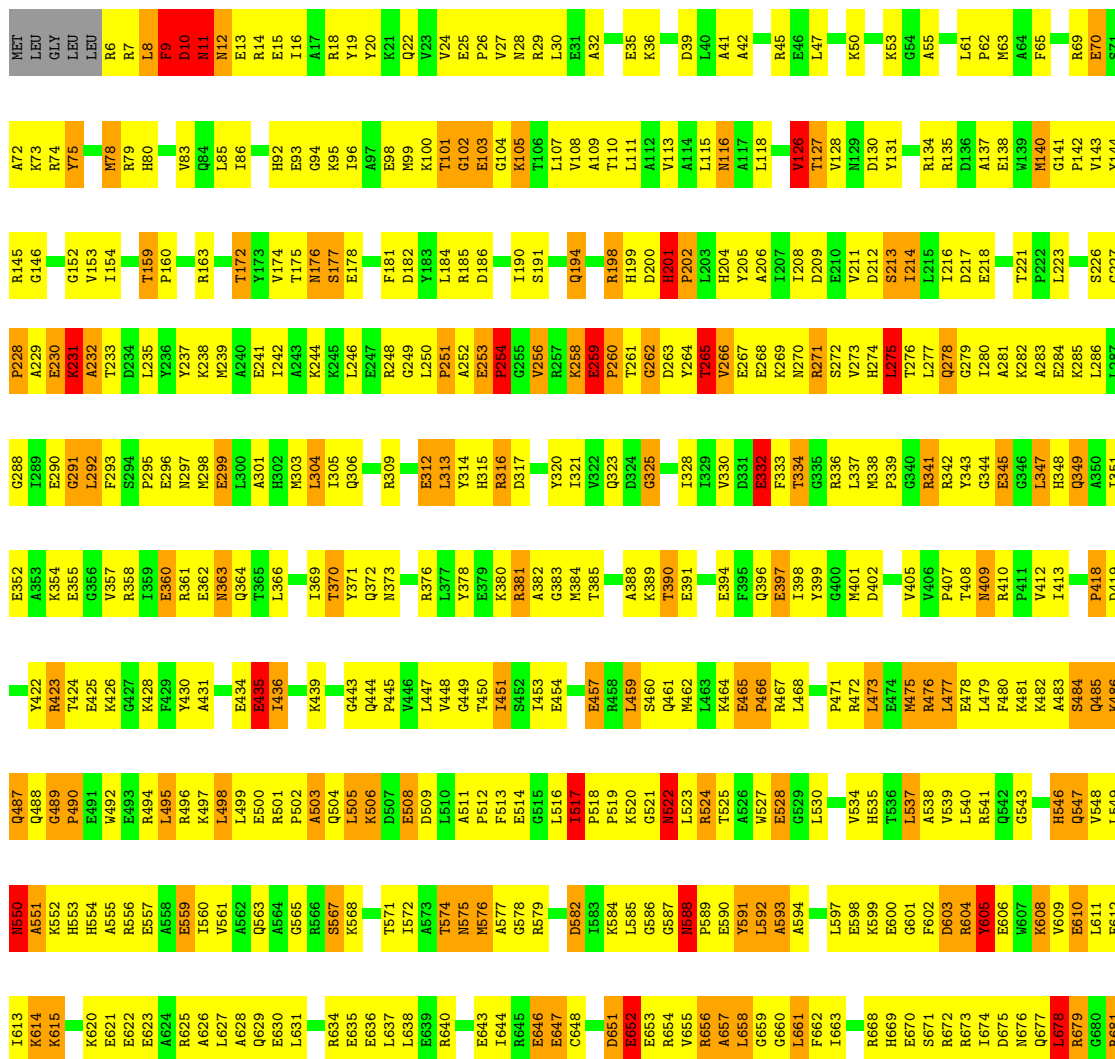
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

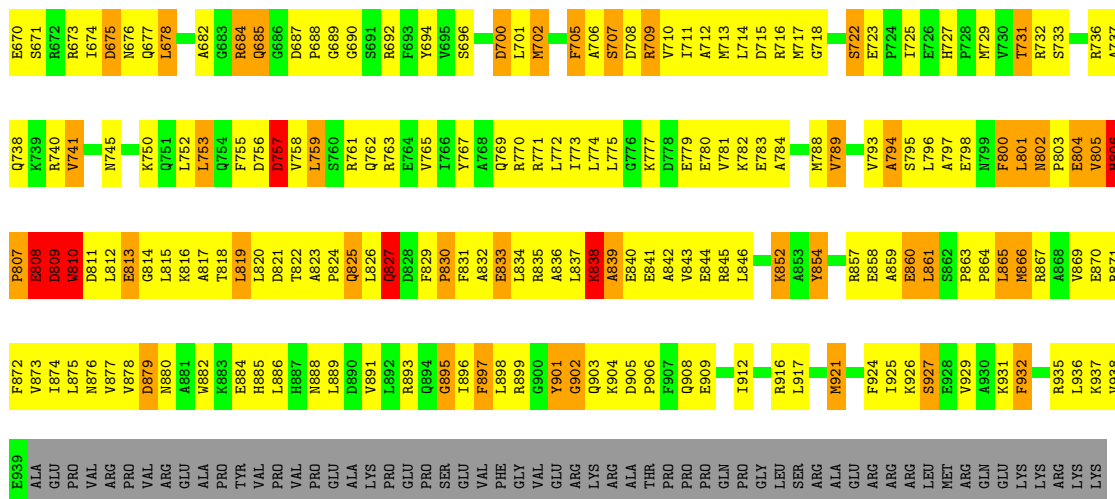
● Molecule 1: Preprotein translocase SecA subunit



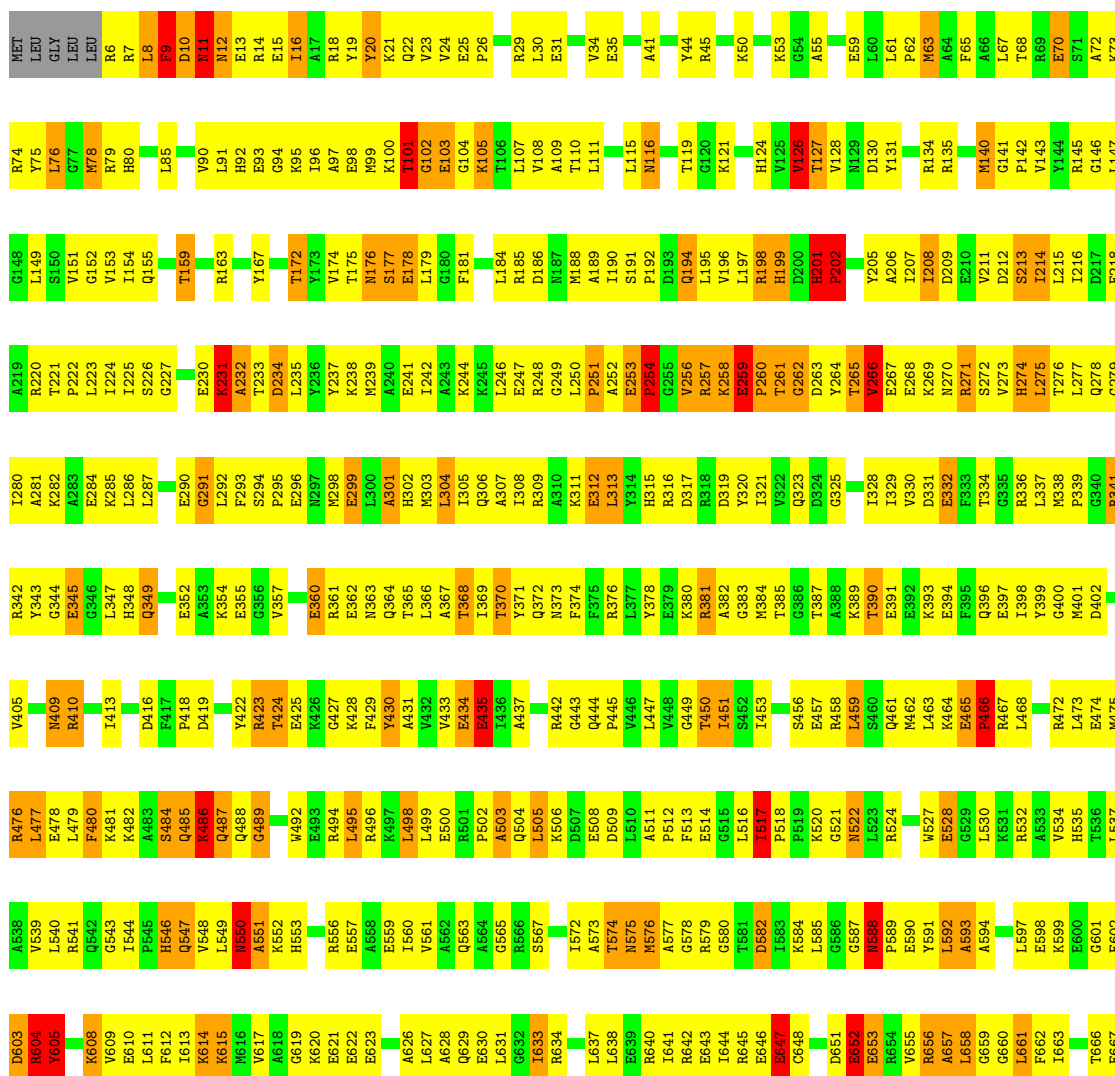
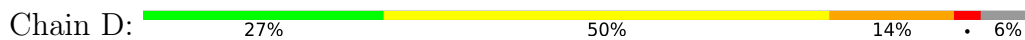


● Molecule 1: Preprotein translocase SecA subunit





● Molecule 1: Preprotein translocase SecA subunit



ARG	A930	L861	A797	T731	R668
GLN	K931	S662	E796	R732	H669
GLU	F932	P863	M799	S733	E670
LYS	L933	P864	F800	I734	S671
LYS	F934	L865	M802	R735	R672
ARG	R935	M866	R803	R736	R673
LYS	L936	R867	R804	A737	I674
LYS	K937	A868	E805	Q738	D675
LYS	V938	V869	V805	K739	N676
ALA	E939	R870	R806	V740	Q677
GLU	R871	F872	P807	V741	L678
GLU	F872	V873	E808	E742	R679
PRO	V873	I874	D809	D743	G680
VAL	I874	L875	K810		R681
ARG	L875	N876	D811	R749	A682
PRO	N876	V877	L812	K750	G683
VAL	V877	V878	E813	R751	R684
ARG	D878	M879	G814	L752	Q685
GLU	D879	M880	L815	L753	Q686
ALA	M880	A881	K816	Q754	D687
PRO	A881	W882	A817	F755	P688
TYR	W882	L886	T818	D756	G689
VAL	L886	H887	L819	D757	G690
PRO	H887		L820	V758	S691
VAL			D821	L759	R692
PRO			T822	S760	F693
GLU	R893		A823	R761	V694
ALA	Q894		P824	V695	Y695
LYS	G895		Q825	R762	S696
PRO	I896		L826	R763	F697
GLU	F897		R827	E764	F697
PRO	R898		D828	V765	D698
SER	R899		F829	I766	D699
GLU	G900		P830	Y767	D700
VAL	Y901		F831	A768	L701
PHE	G902		A832	Q769	M702
GLY	Q903		E833	R770	R703
VAL	K904		L834		L704
GLU	D905		R835	L773	F705
ARG	P906		A836	L774	A706
LYS	F907		L837	L775	S707
ARG	Y910		R838	G776	D708
ALA			A839	K777	R709
THR			E840	D778	V710
PRO	E913		E841	E779	I711
PRO	A914		A842	E780	A712
PRO	T915		V843	V781	M713
GLN				K782	L714
PRO	F918		L846	E783	D715
GLY	N919		W847	A784	D716
LEU	E920		E848	A785	R716
SER	M921		L851	I786	F719
ARG	V922		Y854	G787	F723
ALA	A923			M788	E723
GLU	F924				P724
ARG	I925				I725
ARG	K926				E726
ARG	S927				H727
LEU	E928				P728
MET	V929				M729
					V730
					L796

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	168.62Å 168.62Å 149.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-2.80) 97.5 (40.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.255 0.215 , 0.251	Depositor DCC
R_{free} test set	6730 reflections (5.89%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.038 for -h,-k,l 0.499 for h,-h-k,-l 0.039 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	31502	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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 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	0.72	1/7682 (0.0%)	1.25	89/10350 (0.9%)
1	B	0.75	3/7646 (0.0%)	1.27	92/10302 (0.9%)
1	C	0.71	0/7682	1.25	83/10350 (0.8%)
1	D	0.73	3/7646 (0.0%)	1.27	88/10302 (0.9%)
All	All	0.73	7/30656 (0.0%)	1.26	352/41304 (0.9%)

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	B	0	1
1	C	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	475	MET	SD-CE	6.99	1.97	1.79
1	B	716	ARG	CG-CD	6.74	1.72	1.52
1	D	716	ARG	CG-CD	6.66	1.72	1.52
1	D	434	GLU	C-N	-6.20	1.25	1.33
1	D	151	VAL	CA-CB	5.60	1.59	1.53

The worst 5 of 352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	N-CA-C	13.84	130.94	110.46
1	D	100	LYS	N-CA-C	13.48	125.49	111.07
1	B	100	LYS	N-CA-C	13.41	125.58	110.97
1	D	201	HIS	C-N-CD	-13.17	91.63	120.60
1	B	266	VAL	N-CA-C	-13.09	91.70	109.37

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	591	TYR	Sidechain
1	C	131	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	A	7551	0	7648	771	0
1	B	7515	0	7600	724	0
1	C	7551	0	7648	745	0
1	D	7515	0	7600	835	0
2	A	359	0	0	138	0
2	B	320	0	0	154	0
2	C	344	0	0	149	0
2	D	347	0	0	160	0
All	All	31502	0	30496	3021	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 50.

The worst 5 of 3021 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:D:252:ALA:HB3	1:D:812:LEU:HD11	1.21	1.16
1:D:273:VAL:HG13	1:D:820:LEU:HB2	1.23	1.12
1:C:435:GLU:OE1	1:C:692:ARG:NH1	1.85	1.09
1:A:298:MET:HE1	1:A:873:VAL:HA	1.26	1.09
1:A:269:LYS:HD3	1:A:270:ASN:H	1.08	1.08

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	937/997 (94%)	789 (84%)	101 (11%)	47 (5%)	1	5
1	B	932/997 (94%)	778 (84%)	108 (12%)	46 (5%)	1	6
1	C	937/997 (94%)	784 (84%)	108 (12%)	45 (5%)	2	6
1	D	932/997 (94%)	777 (83%)	107 (12%)	48 (5%)	1	5
All	All	3738/3988 (94%)	3128 (84%)	424 (11%)	186 (5%)	1	5

5 of 186 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	11	ASN
1	A	12	ASN
1	A	231	LYS
1	A	254	PRO

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	788/840 (94%)	656 (83%)	132 (17%)	2	8
1	B	784/840 (93%)	648 (83%)	136 (17%)	2	7
1	C	788/840 (94%)	668 (85%)	120 (15%)	3	10
1	D	784/840 (93%)	649 (83%)	135 (17%)	2	7
All	All	3144/3360 (94%)	2621 (83%)	523 (17%)	2	8

5 of 523 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	605	TYR
1	D	671	SER
1	D	604	ARG
1	D	905	ASP
1	B	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	409	ASN
1	D	11	ASN
1	C	563	GLN
1	C	769	GLN
1	D	124	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

There are no chain breaks in this entry.

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	939/997 (94%)	-1.61	0 100 100	18, 61, 86, 103	0
1	B	934/997 (93%)	-1.60	0 100 100	16, 59, 85, 112	0
1	C	939/997 (94%)	-1.61	0 100 100	20, 61, 88, 102	0
1	D	934/997 (93%)	-1.61	0 100 100	21, 59, 87, 112	0
All	All	3746/3988 (93%)	-1.61	0 100 100	16, 60, 87, 112	0

There are no RSRZ outliers to report.

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.