



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:31 AM UTC

PDB ID : 8KBW / pdb_00008kbw
Title : The crystal structure of syn-copalyl diphosphate synthase from *Oryza sativa*
Authors : Ma, X.L.; Xu, H.F.; Jiang, T.
Deposited on : 2023-08-04
Resolution : 3.49 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
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

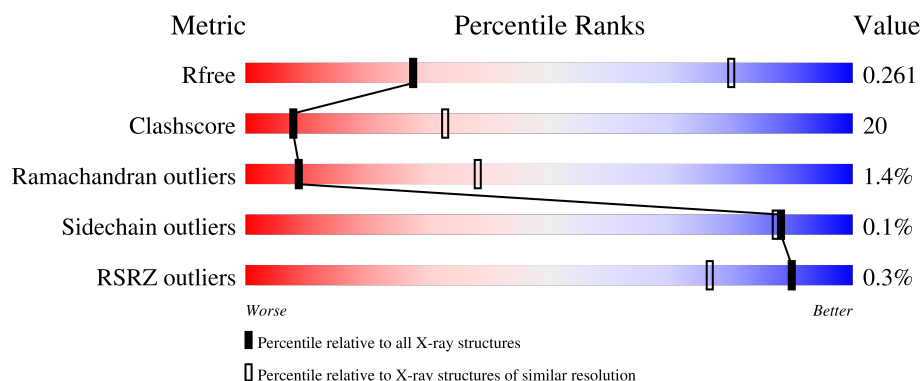
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	775	53% 34% • 11%
1	B	775	54% 32% • 14%
1	C	775	51% 32% • 16%
1	D	775	54% 34% 11%
1	E	775	58% 30% 11%

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Mol	Chain	Length	Quality of chain
1	F	775	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 51%, a yellow segment representing 35%, and a grey segment representing 13%. The percentages are labeled below the corresponding segments.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 32467 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 Syn-copalyl diphosphate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	668	Total	C	N	O	S	0	0	0
			5341	3391	916	1000	34			
1	C	648	Total	C	N	O	S	0	1	0
			5186	3297	892	962	35			
1	E	688	Total	C	N	O	S	0	0	0
			5504	3492	944	1033	35			
1	D	688	Total	C	N	O	S	0	0	0
			5504	3492	944	1033	35			
1	F	677	Total	C	N	O	S	0	0	0
			5421	3439	928	1019	35			
1	A	689	Total	C	N	O	S	0	0	0
			5511	3496	945	1035	35			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	768	GLU	-	expression tag	UNP Q0JF02
B	769	PHE	-	expression tag	UNP Q0JF02
B	770	HIS	-	expression tag	UNP Q0JF02
B	771	HIS	-	expression tag	UNP Q0JF02
B	772	HIS	-	expression tag	UNP Q0JF02
B	773	HIS	-	expression tag	UNP Q0JF02
B	774	HIS	-	expression tag	UNP Q0JF02
B	775	HIS	-	expression tag	UNP Q0JF02
C	768	GLU	-	expression tag	UNP Q0JF02
C	769	PHE	-	expression tag	UNP Q0JF02
C	770	HIS	-	expression tag	UNP Q0JF02
C	771	HIS	-	expression tag	UNP Q0JF02
C	772	HIS	-	expression tag	UNP Q0JF02
C	773	HIS	-	expression tag	UNP Q0JF02
C	774	HIS	-	expression tag	UNP Q0JF02
C	775	HIS	-	expression tag	UNP Q0JF02
E	768	GLU	-	expression tag	UNP Q0JF02

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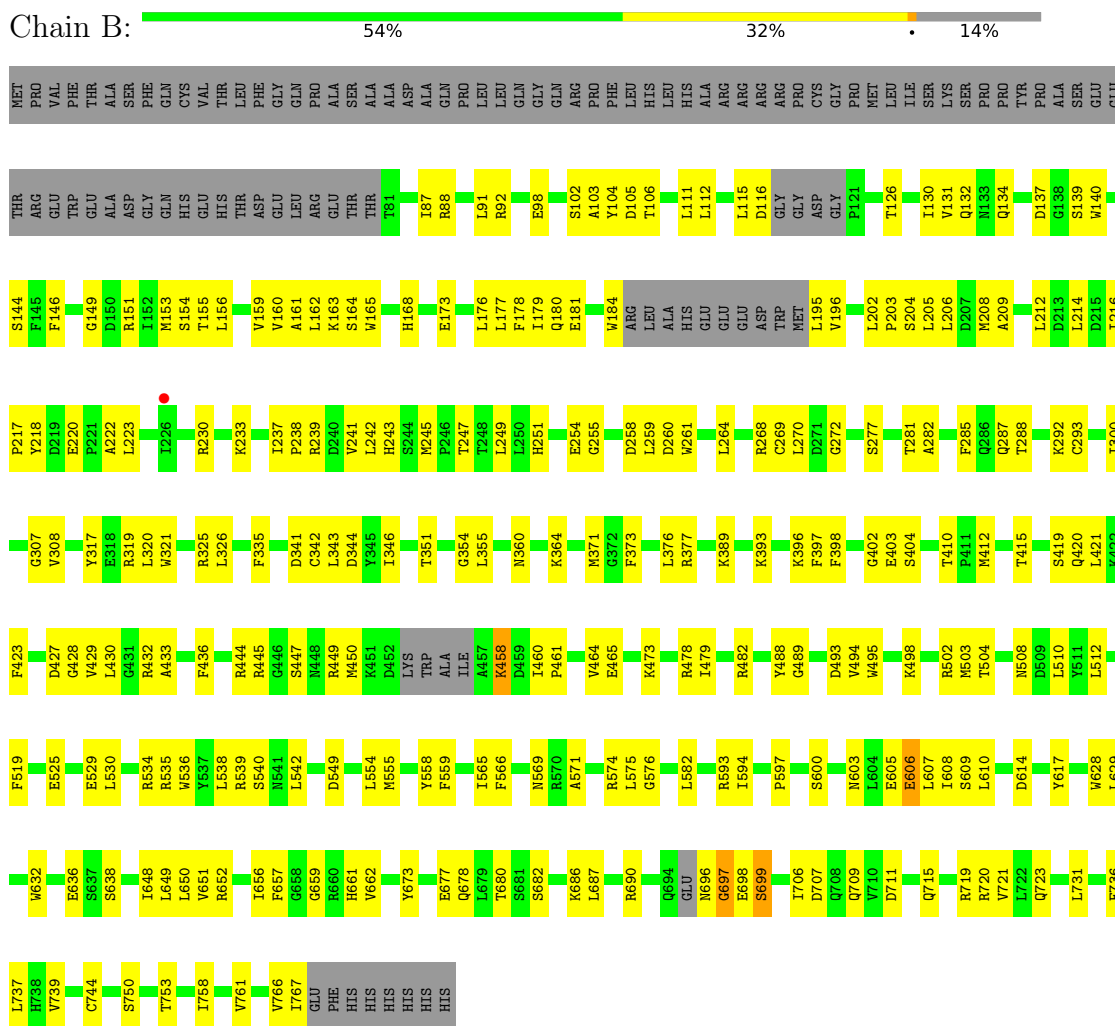
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Chain	Residue	Modelled	Actual	Comment	Reference
E	769	PHE	-	expression tag	UNP Q0JF02
E	770	HIS	-	expression tag	UNP Q0JF02
E	771	HIS	-	expression tag	UNP Q0JF02
E	772	HIS	-	expression tag	UNP Q0JF02
E	773	HIS	-	expression tag	UNP Q0JF02
E	774	HIS	-	expression tag	UNP Q0JF02
E	775	HIS	-	expression tag	UNP Q0JF02
D	768	GLU	-	expression tag	UNP Q0JF02
D	769	PHE	-	expression tag	UNP Q0JF02
D	770	HIS	-	expression tag	UNP Q0JF02
D	771	HIS	-	expression tag	UNP Q0JF02
D	772	HIS	-	expression tag	UNP Q0JF02
D	773	HIS	-	expression tag	UNP Q0JF02
D	774	HIS	-	expression tag	UNP Q0JF02
D	775	HIS	-	expression tag	UNP Q0JF02
F	768	GLU	-	expression tag	UNP Q0JF02
F	769	PHE	-	expression tag	UNP Q0JF02
F	770	HIS	-	expression tag	UNP Q0JF02
F	771	HIS	-	expression tag	UNP Q0JF02
F	772	HIS	-	expression tag	UNP Q0JF02
F	773	HIS	-	expression tag	UNP Q0JF02
F	774	HIS	-	expression tag	UNP Q0JF02
F	775	HIS	-	expression tag	UNP Q0JF02
A	768	GLU	-	expression tag	UNP Q0JF02
A	769	PHE	-	expression tag	UNP Q0JF02
A	770	HIS	-	expression tag	UNP Q0JF02
A	771	HIS	-	expression tag	UNP Q0JF02
A	772	HIS	-	expression tag	UNP Q0JF02
A	773	HIS	-	expression tag	UNP Q0JF02
A	774	HIS	-	expression tag	UNP Q0JF02
A	775	HIS	-	expression tag	UNP Q0JF02

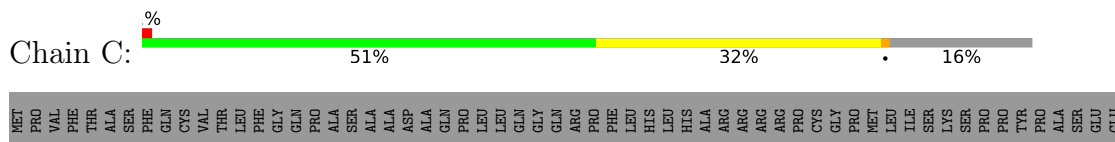
3 Residue-property plots

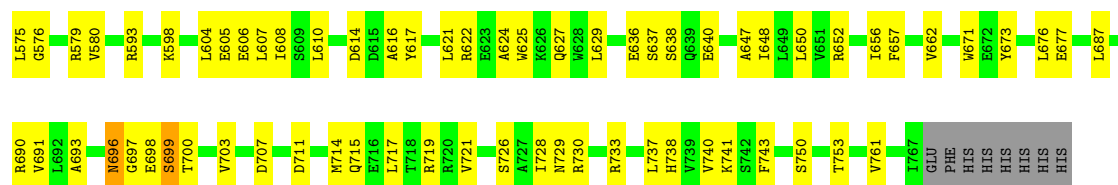
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



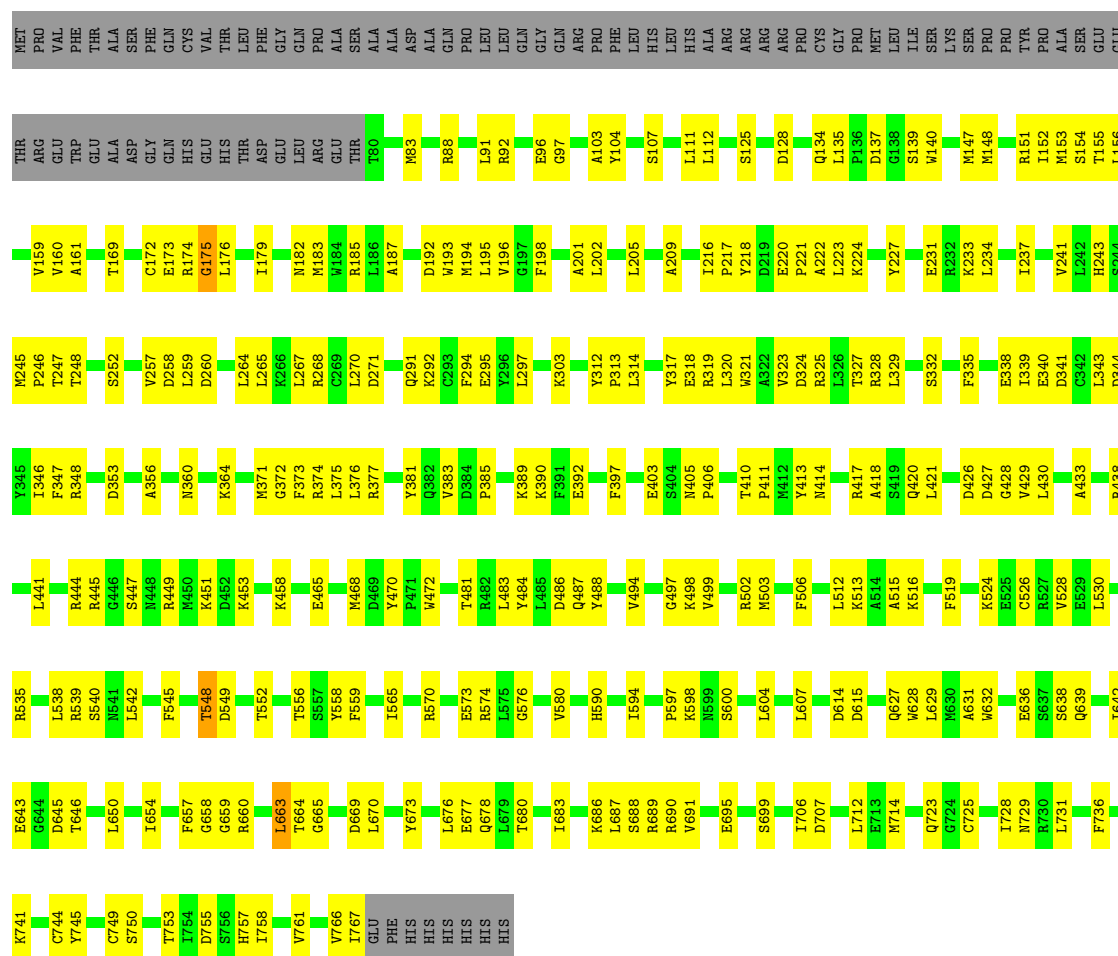
- Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic





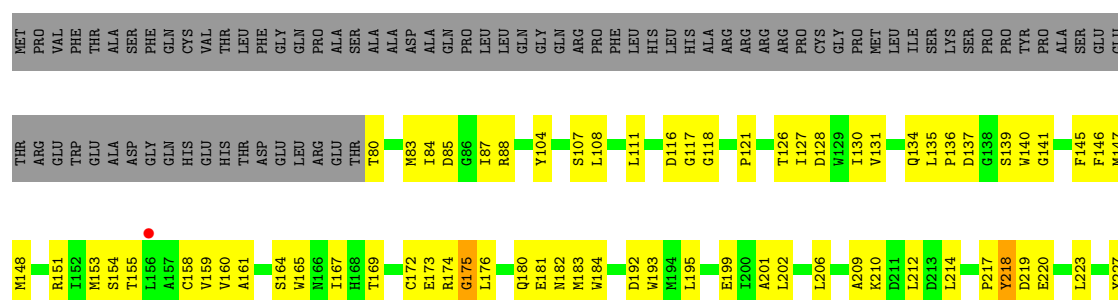
- Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

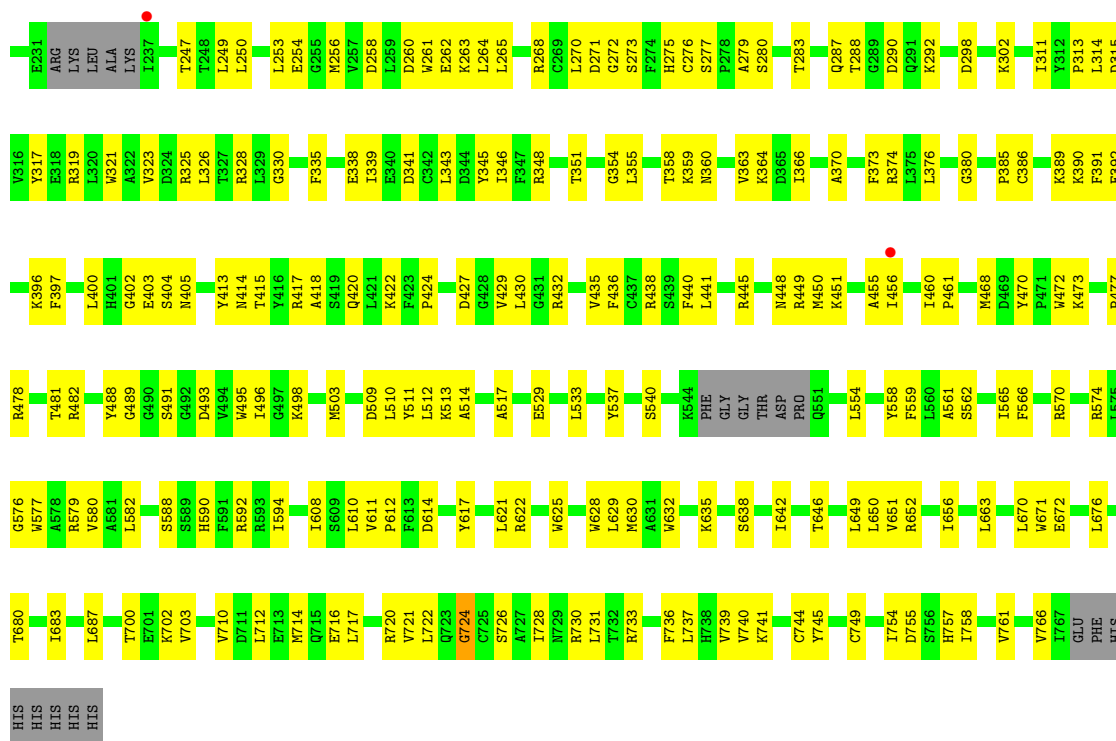
Chain D: 54% 34% 11%



- Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

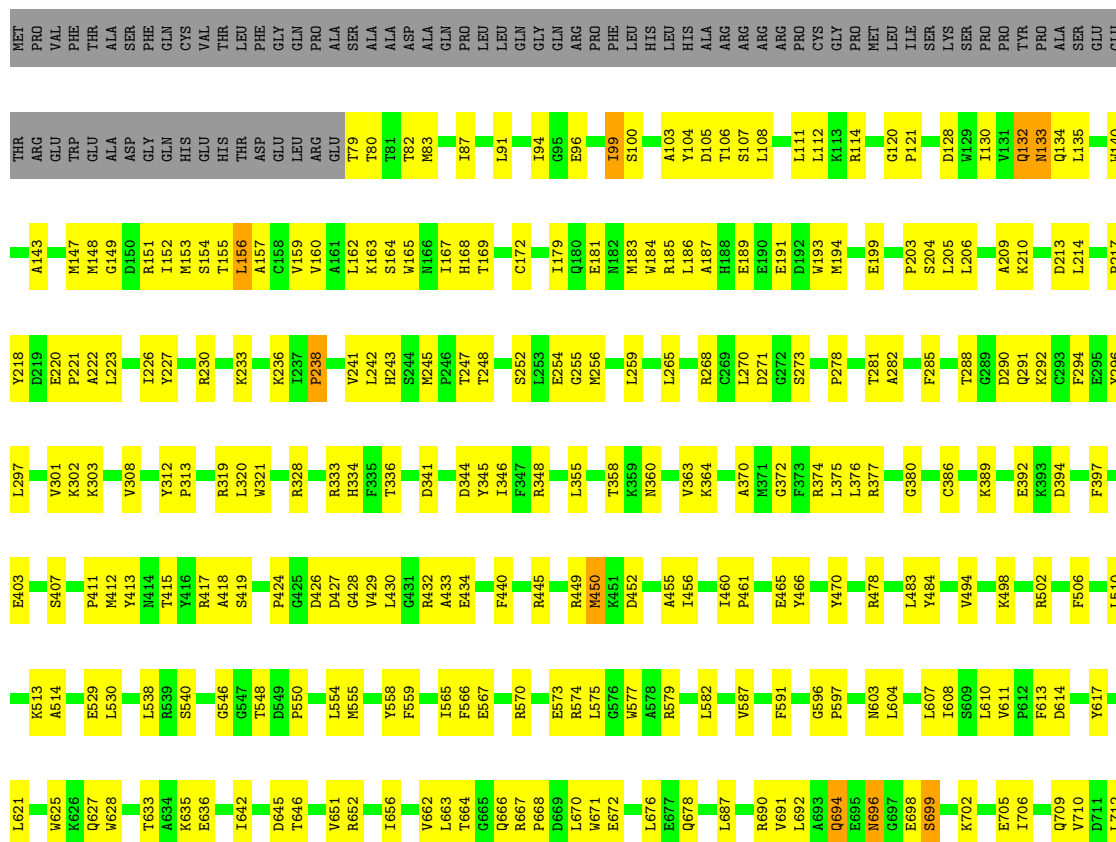
Chain F: 51% 35% 13%





• Molecule 1: Syn-copalyl diphosphate synthase, chloroplastic

Chain A: 53% 34% 11%



E713	M714	Q715	E716	R720	Y721	L722	S726	A727	I728	L731	I732	R733	E734	T735	F736	L737	K741	C744	Y745	Y748	C749	S750	T753	I754	D755	S756	H757	I758	I767	GLU	PHE	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	129.70Å 174.34Å 296.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.62 – 3.49 97.62 – 3.49	Depositor EDS
% Data completeness (in resolution range)	96.5 (97.62-3.49) 95.3 (97.62-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.201 , 0.263 0.199 , 0.261	Depositor DCC
R_{free} test set	2000 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32467	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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	0.60	0/5634	0.87	2/7625 (0.0%)
1	B	0.49	0/5455	0.78	0/7375
1	C	0.49	0/5297	0.78	1/7155 (0.0%)
1	D	0.47	1/5627 (0.0%)	0.72	0/7615
1	E	0.53	0/5627	0.78	0/7615
1	F	0.45	0/5540	0.76	0/7496
All	All	0.51	1/33180 (0.0%)	0.78	3/44881 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	548	THR	CA-C	5.66	1.60	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	689	ARG	N-CA-C	-6.35	107.39	114.62
1	A	132	GLN	CA-C-N	-5.50	115.61	123.20
1	A	132	GLN	C-N-CA	-5.50	115.61	123.20

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	5511	0	5420	236	0
1	B	5341	0	5268	210	0
1	C	5186	0	5140	213	0
1	D	5504	0	5413	218	0
1	E	5504	0	5413	192	0
1	F	5421	0	5323	239	0
All	All	32467	0	31977	1274	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 20.

The worst 5 of 1274 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:608:ILE:HD11	1:E:621:LEU:HD22	1.34	1.08
1:A:156:LEU:HD11	1:A:205:LEU:HG	1.38	1.04
1:F:460:ILE:HG23	1:F:461:PRO:HD3	1.49	0.94
1:F:441:LEU:HB2	1:F:468:MET:HE3	1.50	0.94
1:B:606:GLU:O	1:B:608:ILE:N	2.01	0.92

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	687/775 (89%)	621 (90%)	56 (8%)	10 (2%)	8	37
1	B	658/775 (85%)	611 (93%)	37 (6%)	10 (2%)	8	37
1	C	635/775 (82%)	571 (90%)	52 (8%)	12 (2%)	6	33
1	D	686/775 (88%)	637 (93%)	41 (6%)	8 (1%)	10	41
1	E	686/775 (88%)	630 (92%)	49 (7%)	7 (1%)	12	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	671/775 (87%)	605 (90%)	57 (8%)	9 (1%)	9	39
All	All	4023/4650 (86%)	3675 (91%)	292 (7%)	56 (1%)	9	38

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	403	GLU
1	B	607	LEU
1	B	697	GLY
1	C	183	MET
1	C	664	THR

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	598/672 (89%)	596 (100%)	2 (0%)	86	83
1	B	582/672 (87%)	582 (100%)	0	100	100
1	C	565/672 (84%)	565 (100%)	0	100	100
1	D	597/672 (89%)	597 (100%)	0	100	100
1	E	597/672 (89%)	596 (100%)	1 (0%)	87	85
1	F	589/672 (88%)	589 (100%)	0	100	100
All	All	3528/4032 (88%)	3525 (100%)	3 (0%)	88	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	196	VAL
1	A	133	ASN
1	A	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	603	ASN
1	F	675	GLN
1	A	448	ASN
1	E	442	GLN
1	E	420	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 [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	689/775 (88%)	-0.61	0 100 100	32, 56, 100, 127	0
1	B	668/775 (86%)	-0.47	1 (0%) 92 86	34, 76, 118, 132	0
1	C	648/775 (83%)	-0.23	9 (1%) 73 48	31, 85, 150, 177	1 (0%)
1	D	688/775 (88%)	-0.38	0 100 100	41, 84, 138, 160	0
1	E	688/775 (88%)	-0.55	0 100 100	41, 67, 111, 131	0
1	F	677/775 (87%)	-0.12	3 (0%) 88 72	50, 95, 145, 169	0
All	All	4058/4650 (87%)	-0.39	13 (0%) 90 76	31, 76, 135, 177	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	ILE	3.2
1	C	152	ILE	2.9
1	C	221	PRO	2.6
1	F	456	ILE	2.6
1	C	209	ALA	2.5

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.