



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:51 pm BST

PDB ID : 6QL7
Title : Structure of fatty acid synthase complex with bound gamma subunit from *Saccharomyces cerevisiae* at 4.6 angstrom
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.
Deposited on : 2019-01-31
Resolution : 4.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

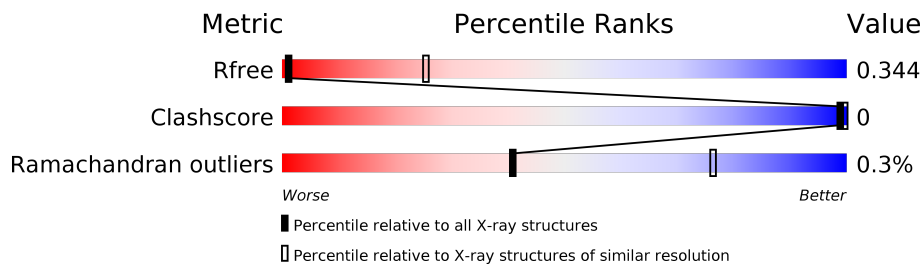
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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.



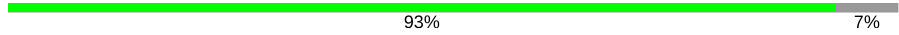
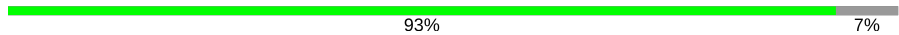


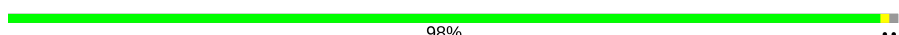
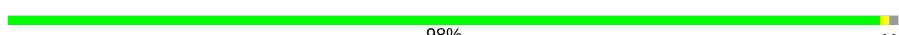
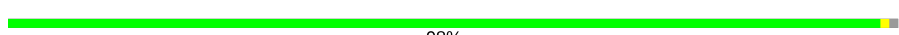




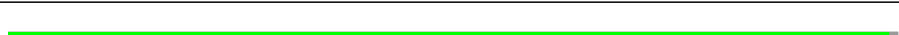


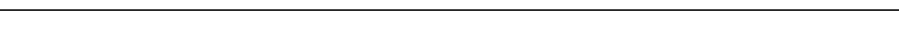
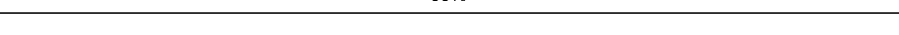

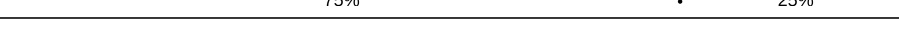







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1887	92% 7%
1	B	1887	92% 7%
1	C	1887	92% 7%
1	D	1887	92% 7%
1	E	1887	92% 7%
1	F	1887	92% 7%
1	a	1887	93% 7%
1	b	1887	93% 7%
1	c	1887	93% 7%



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Mol	Chain	Length	Quality of chain
1	d	1887	 93% 7%
1	e	1887	 93% 7%
1	f	1887	 93% 7%
2	G	2051	 98% ..
2	H	2051	 98% ..
2	I	2051	 98% ..
2	J	2051	 98% ..
2	K	2051	 98% ..
2	L	2051	 98% ..
2	g	2051	 99% .
2	h	2051	 99% .
2	i	2051	 99% .
2	j	2051	 99% .
2	k	2051	 99% .
2	l	2051	 99% .
3	M	150	 75% . 25%
3	N	150	 75% . 25%
3	O	150	 74% . 25%
3	P	150	 74% . 25%
3	Q	150	 74% . 25%
3	R	150	 74% . 25%
3	m	150	 75% . 25%
3	n	150	 75% . 25%
3	o	150	 75% . 25%
3	p	150	 75% . 25%

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Mol	Chain	Length	Quality of chain
3	q	150	 75% 25%
3	r	150	 75% 25%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 231252 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	1760	8667	5147	1760	1760	0	0	0
1	B	1760	8667	5147	1760	1760	0	0	0
1	C	1760	8667	5147	1760	1760	0	0	0
1	D	1760	8667	5147	1760	1760	0	0	0
1	E	1760	8667	5147	1760	1760	0	0	0
1	F	1760	8667	5147	1760	1760	0	0	0
1	a	1760	8667	5147	1760	1760	0	0	0
1	b	1760	8667	5147	1760	1760	0	0	0
1	c	1760	8667	5147	1760	1760	0	0	0
1	d	1760	8667	5147	1760	1760	0	0	0
1	e	1760	8667	5147	1760	1760	0	0	0
1	f	1760	8667	5147	1760	1760	0	0	0

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	G	2036	10046	5974	2036	2036	0	0	0
2	H	2036	10046	5974	2036	2036	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	J	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	K	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	L	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	g	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	h	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	i	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	j	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	k	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0
2	l	2036	Total 10046	C 5974	N 2036	O 2036	0	0	0

- Molecule 3 is a protein called Translation machinery-associated protein 17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	113	Total 558	C 332	N 113	O 113	0	0	0
3	N	113	Total 558	C 332	N 113	O 113	0	0	0
3	O	113	Total 558	C 332	N 113	O 113	0	0	0
3	P	113	Total 558	C 332	N 113	O 113	0	0	0
3	Q	113	Total 558	C 332	N 113	O 113	0	0	0
3	R	113	Total 558	C 332	N 113	O 113	0	0	0
3	m	113	Total 558	C 332	N 113	O 113	0	0	0
3	n	113	Total 558	C 332	N 113	O 113	0	0	0
3	o	113	Total 558	C 332	N 113	O 113	0	0	0

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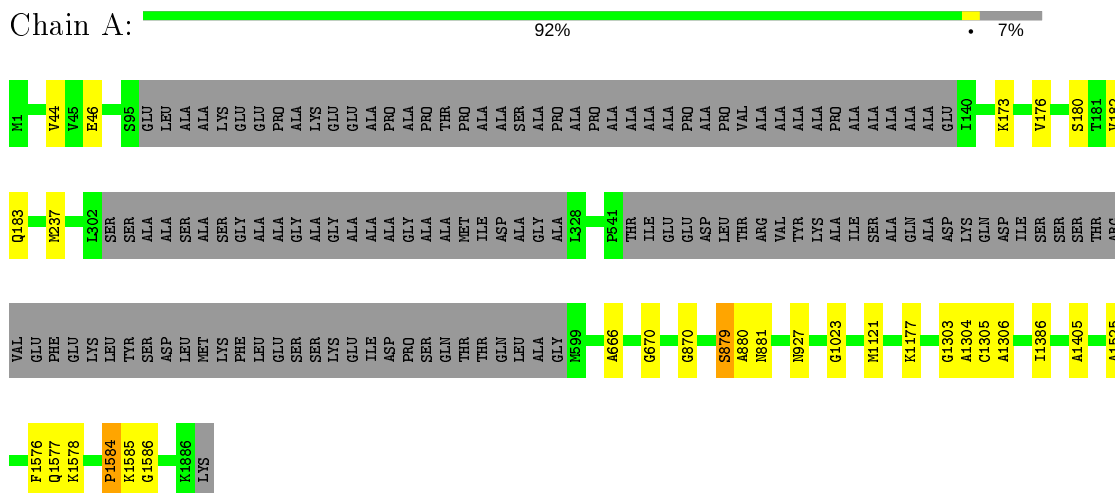
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	p	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	q	113	Total	C	N	O	0	0	0
			558	332	113	113			
3	r	113	Total	C	N	O	0	0	0
			558	332	113	113			

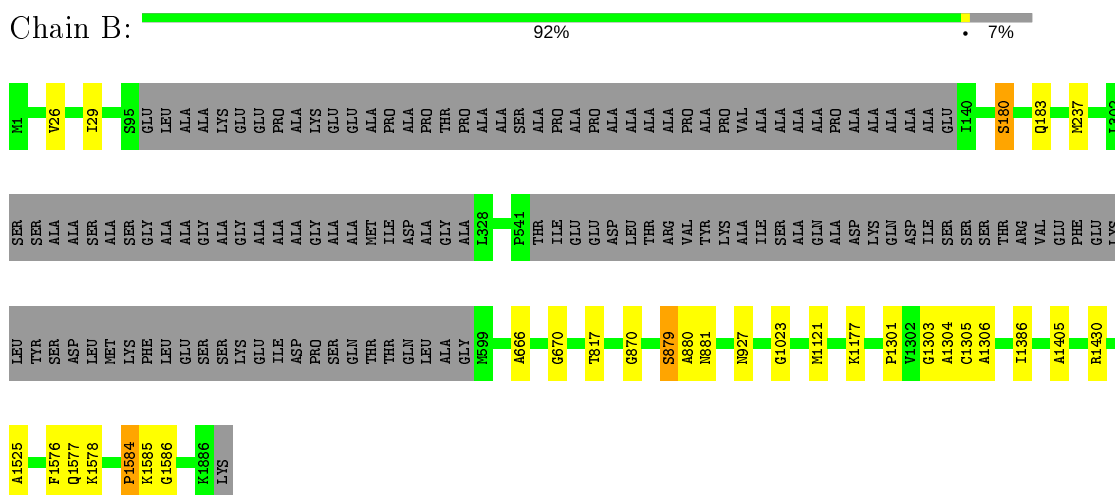
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Fatty acid synthase subunit alpha

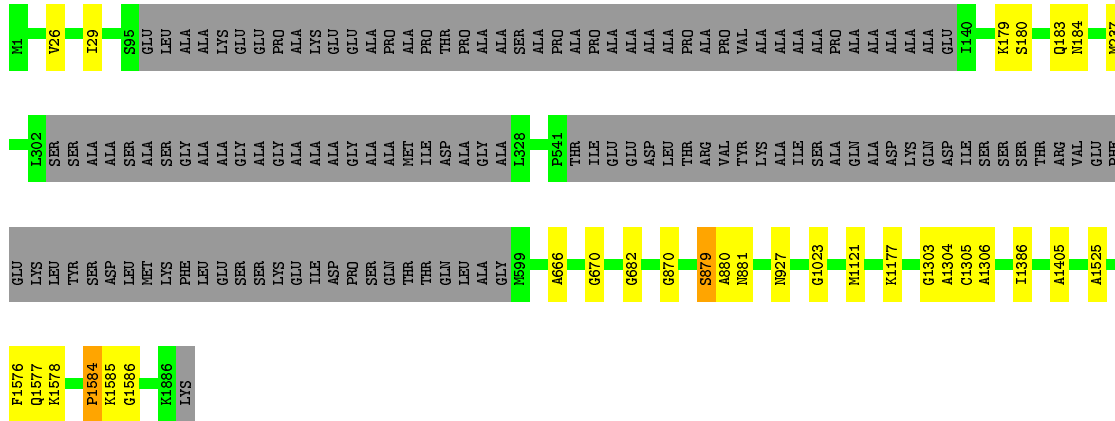


- Molecule 1: Fatty acid synthase subunit alpha



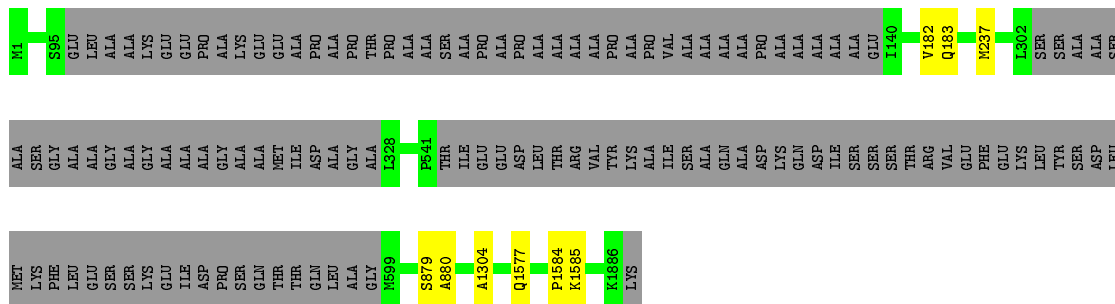
- Molecule 1: Fatty acid synthase subunit alpha





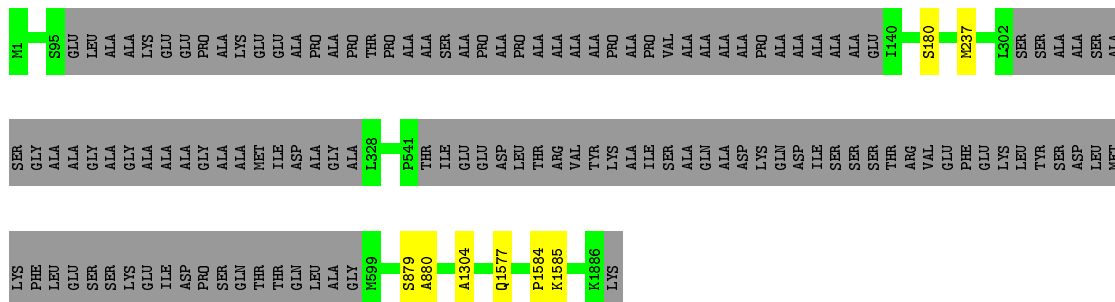
- Molecule 1: Fatty acid synthase subunit alpha

Chain a: 93% 7%



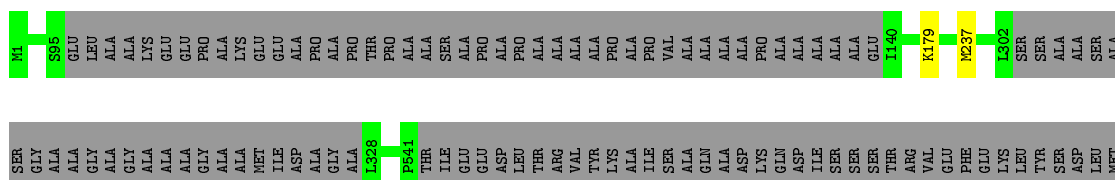
- Molecule 1: Fatty acid synthase subunit alpha

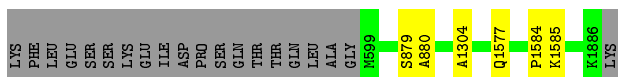
Chain b: 93% 7%



- Molecule 1: Fatty acid synthase subunit alpha

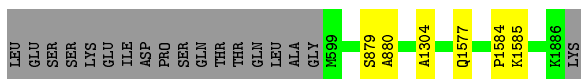
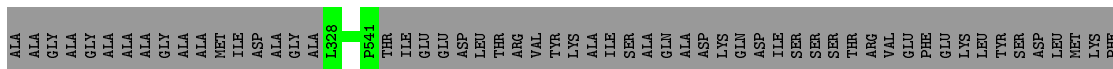
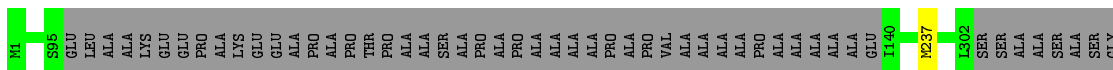
Chain c: 93% 7%





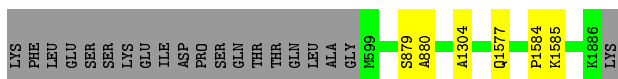
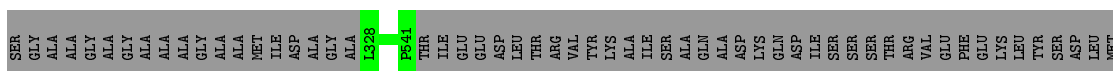
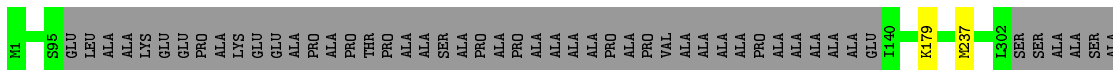
- Molecule 1: Fatty acid synthase subunit alpha

Chain d: 93% 7%



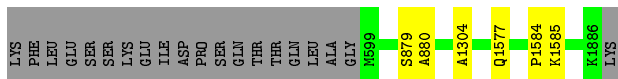
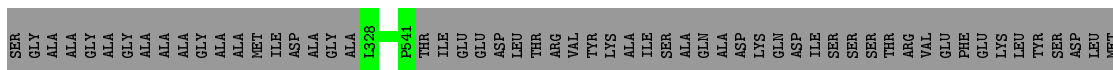
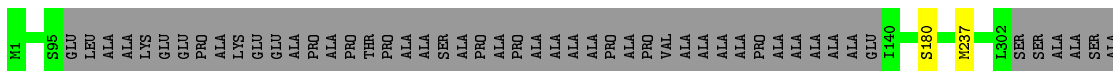
- Molecule 1: Fatty acid synthase subunit alpha

Chain e: 93% 7%



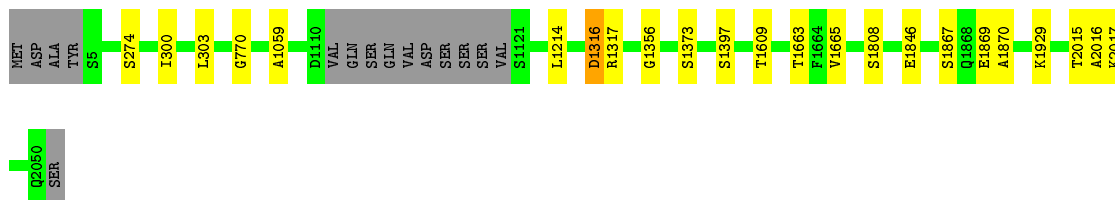
- Molecule 1: Fatty acid synthase subunit alpha

Chain f: 93% 7%



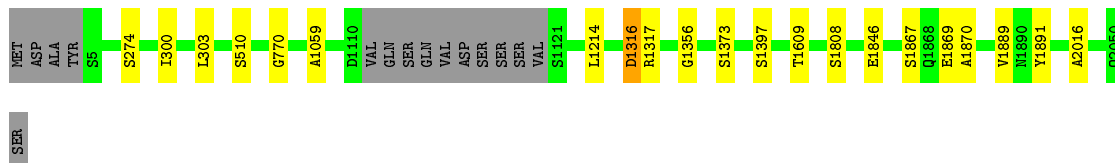
- Molecule 2: Fatty acid synthase subunit beta

Chain G: 98% ..



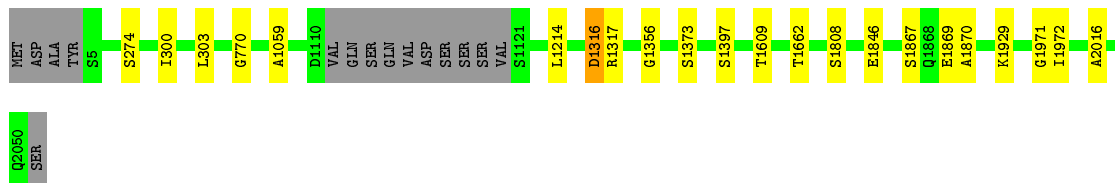
- Molecule 2: Fatty acid synthase subunit beta

Chain H: 98%



- Molecule 2: Fatty acid synthase subunit beta

Chain I: 98%



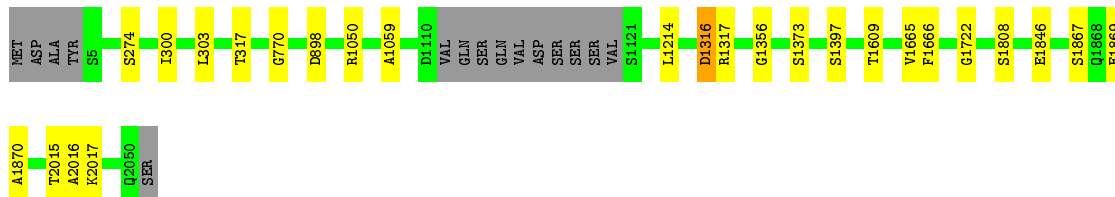
- Molecule 2: Fatty acid synthase subunit beta

Chain J: 98%



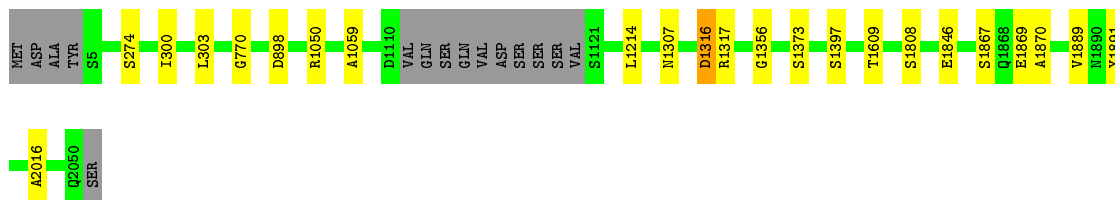
- Molecule 2: Fatty acid synthase subunit beta

Chain K: 98%



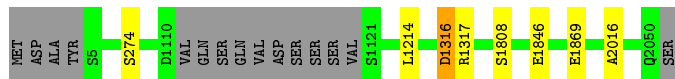
- Molecule 2: Fatty acid synthase subunit beta

Chain L: 98%



- Molecule 2: Fatty acid synthase subunit beta

Chain g: 99%



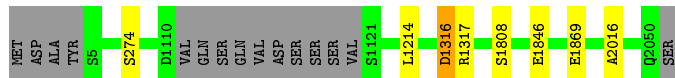
- Molecule 2: Fatty acid synthase subunit beta

Chain h: 99%



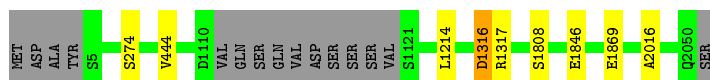
- Molecule 2: Fatty acid synthase subunit beta

Chain i: 99%



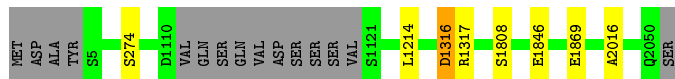
- Molecule 2: Fatty acid synthase subunit beta

Chain j: 99%



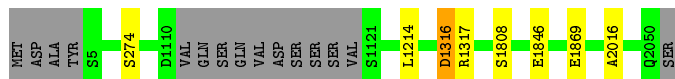
- Molecule 2: Fatty acid synthase subunit beta

Chain k: 99%



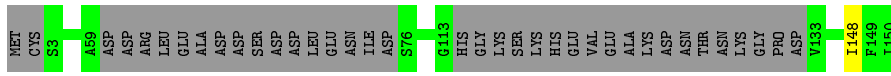
- Molecule 2: Fatty acid synthase subunit beta

Chain l: 99%



- Molecule 3: Translation machinery-associated protein 17

Chain M:  75% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain N:  75% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain O:  74% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain P:  74% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain Q:  74% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain R:  74% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain m:  75% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain n:  75% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain o:  75% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain p:  75% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain q:  75% 25%



- Molecule 3: Translation machinery-associated protein 17

Chain r:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	234.92Å 430.31Å 422.61Å 90.00° 97.01° 90.00°	Depositor
Resolution (Å)	192.50 – 4.60 192.51 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (192.50-4.60) 99.6 (192.51-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 4.66Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.252 , 0.310 0.327 , 0.344	Depositor DCC
R_{free} test set	22715 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	218.0	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , 401.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	231252	wwPDB-VP
Average B, all atoms (Å ²)	256.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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	0.80	1/8663 (0.0%)	0.83	0/12042
1	B	0.81	2/8663 (0.0%)	0.83	0/12042
1	C	0.81	0/8663	0.83	0/12042
1	D	0.80	1/8663 (0.0%)	0.83	0/12042
1	E	0.81	2/8663 (0.0%)	0.83	1/12042 (0.0%)
1	F	0.81	0/8663	0.83	0/12042
1	a	0.80	0/8663	0.83	0/12042
1	b	0.81	1/8663 (0.0%)	0.83	0/12042
1	c	0.81	0/8663	0.83	0/12042
1	d	0.81	0/8663	0.83	0/12042
1	e	0.81	0/8663	0.83	0/12042
1	f	0.80	1/8663 (0.0%)	0.83	0/12042
2	G	0.81	0/10042	0.83	0/13972
2	H	0.81	0/10042	0.82	0/13972
2	I	0.81	0/10041	0.83	0/13969
2	J	0.80	0/10042	0.83	0/13972
2	K	0.81	0/10042	0.83	0/13972
2	L	0.81	0/10042	0.83	0/13972
2	g	0.81	0/10042	0.83	0/13972
2	h	0.81	0/10042	0.83	0/13972
2	i	0.81	0/10042	0.82	0/13972
2	j	0.81	0/10042	0.83	0/13972
2	k	0.81	0/10042	0.83	0/13972
2	l	0.81	0/10042	0.83	0/13972
3	M	0.86	0/555	0.81	0/768
3	N	0.86	0/555	0.82	0/768
3	O	0.86	0/555	0.81	0/768
3	P	0.86	0/555	0.82	0/768
3	Q	0.86	0/555	0.81	0/768
3	R	0.86	0/555	0.81	0/768
3	m	0.86	0/555	0.81	0/768
3	n	0.86	0/555	0.81	0/768
3	o	0.86	0/555	0.81	0/768
3	p	0.86	0/555	0.81	0/768

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	q	0.86	0/555	0.81	0/768
3	r	0.86	0/555	0.81	0/768
All	All	0.81	8/231119 (0.0%)	0.83	1/321381 (0.0%)

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	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	a	0	3
1	b	0	3
1	c	0	3
1	d	0	3
1	e	0	3
1	f	0	3
2	G	0	1
2	H	0	1
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
2	g	0	1
2	h	0	1
2	i	0	1
2	j	0	1
2	k	0	1
2	l	0	1
All	All	0	48

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	SER	C-O	5.97	1.34	1.23
1	E	180	SER	CA-CB	5.89	1.61	1.52
1	B	180	SER	CA-CB	5.82	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	180	SER	CA-CB	5.75	1.61	1.52
1	D	180	SER	CA-CB	5.61	1.61	1.52
1	f	180	SER	CA-CB	5.59	1.61	1.52
1	A	180	SER	CA-CB	5.38	1.61	1.52
1	E	180	SER	C-O	5.26	1.33	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	178	GLY	C-N-CA	5.54	135.56	121.70

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1584	PRO	Peptide
1	A	237	MET	Peptide
1	A	879	SER	Peptide
1	B	1584	PRO	Peptide
1	B	237	MET	Peptide
1	B	879	SER	Peptide
1	C	1584	PRO	Peptide
1	C	237	MET	Peptide
1	C	879	SER	Peptide
1	D	1584	PRO	Peptide
1	D	237	MET	Peptide
1	D	879	SER	Peptide
1	E	1584	PRO	Peptide
1	E	237	MET	Peptide
1	E	879	SER	Peptide
1	F	1584	PRO	Peptide
1	F	237	MET	Peptide
1	F	879	SER	Peptide
2	G	1316	ASP	Peptide
2	H	1316	ASP	Peptide
2	I	1316	ASP	Peptide
2	J	1316	ASP	Peptide
2	K	1316	ASP	Peptide
2	L	1316	ASP	Peptide
1	a	1584	PRO	Peptide
1	a	237	MET	Peptide
1	a	879	SER	Peptide

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Mol	Chain	Res	Type	Group
1	b	1584	PRO	Peptide
1	b	237	MET	Peptide
1	b	879	SER	Peptide
1	c	1584	PRO	Peptide
1	c	237	MET	Peptide
1	c	879	SER	Peptide
1	d	1584	PRO	Peptide
1	d	237	MET	Peptide
1	d	879	SER	Peptide
1	e	1584	PRO	Peptide
1	e	237	MET	Peptide
1	e	879	SER	Peptide
1	f	1584	PRO	Peptide
1	f	237	MET	Peptide
1	f	879	SER	Peptide
2	g	1316	ASP	Peptide
2	h	1316	ASP	Peptide
2	i	1316	ASP	Peptide
2	j	1316	ASP	Peptide
2	k	1316	ASP	Peptide
2	l	1316	ASP	Peptide

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	8667	0	4008	14	0
1	B	8667	0	4008	17	0
1	C	8667	0	4008	16	0
1	D	8667	0	4008	21	0
1	E	8667	0	4008	14	0
1	F	8667	0	4008	20	0
1	a	8667	0	4008	0	0
1	b	8667	0	4008	0	0
1	c	8667	0	4008	0	0
1	d	8667	0	4008	0	0
1	e	8667	0	4008	0	0
1	f	8667	0	4008	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	10046	0	4474	8	1
2	H	10046	0	4474	9	0
2	I	10046	0	4473	9	3
2	J	10046	0	4474	7	0
2	K	10046	0	4474	11	0
2	L	10046	0	4474	9	0
2	g	10046	0	4474	0	0
2	h	10046	0	4474	0	1
2	i	10046	0	4474	0	0
2	j	10046	0	4474	0	3
2	k	10046	0	4474	0	0
2	l	10046	0	4474	0	0
3	M	558	0	252	0	0
3	N	558	0	252	0	0
3	O	558	0	252	1	0
3	P	558	0	252	1	0
3	Q	558	0	252	1	0
3	R	558	0	252	1	0
3	m	558	0	252	0	0
3	n	558	0	252	0	0
3	o	558	0	252	0	0
3	p	558	0	252	0	0
3	q	558	0	252	0	0
3	r	558	0	252	0	0
All	All	231252	0	104807	138	4

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 0.

All (138) 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:F:180:SER:HA	1:F:183:GLN:CB	1.69	1.19
2:I:1971:GLY:C	2:I:1972:ILE:N	2.00	1.14
1:F:180:SER:O	1:F:184:ASN:N	1.87	1.07
1:B:180:SER:HA	1:B:183:GLN:CB	1.94	0.97
1:D:180:SER:HA	1:D:183:GLN:CB	1.99	0.93
1:D:180:SER:O	1:D:184:ASN:N	2.04	0.89
1:D:173:LYS:O	1:D:176:VAL:O	3.17	0.83
1:F:180:SER:CA	1:F:183:GLN:CB	2.57	0.79
2:I:1971:GLY:C	2:I:1972:ILE:CA	2.57	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:682:GLY:HA2	3:R:136:ASP:HA	1.73	0.69
1:B:180:SER:CA	1:B:183:GLN:CB	2.72	0.66
1:D:682:GLY:HA2	3:P:136:ASP:HA	1.76	0.66
1:C:181:THR:CB	2:H:510:SER:CB	4.16	0.64
1:C:682:GLY:HA2	3:O:136:ASP:HA	2.59	0.62
1:E:682:GLY:HA2	3:Q:136:ASP:HA	2.17	0.61
1:D:180:SER:CA	1:D:183:GLN:CB	2.76	0.60
1:D:43:ARG:O	2:J:1662:THR:HA	2.60	0.60
1:B:29:ILE:N	2:H:1891:TYR:O	2.71	0.59
1:A:173:LYS:O	1:A:176:VAL:O	3.17	0.59
1:A:46:GLU:HA	2:G:1665:VAL:O	2.06	0.56
1:D:180:SER:O	1:D:183:GLN:CB	2.54	0.56
1:A:182:VAL:O	1:A:183:GLN:CB	4.34	0.55
1:F:180:SER:O	1:F:183:GLN:CB	2.55	0.55
1:B:817:THR:O	2:K:1722:GLY:N	3.35	0.54
1:F:180:SER:O	1:F:183:GLN:CA	2.55	0.54
1:C:1303:GLY:O	1:C:1306:ALA:N	2.41	0.53
1:A:1303:GLY:O	1:A:1306:ALA:N	2.42	0.53
1:E:1303:GLY:O	1:E:1306:ALA:N	2.42	0.53
1:D:1303:GLY:O	1:D:1306:ALA:N	2.42	0.53
1:B:1303:GLY:O	1:B:1306:ALA:N	2.42	0.53
1:C:43:ARG:O	2:I:1662:THR:HA	2.12	0.53
1:D:180:SER:O	1:D:183:GLN:CA	2.57	0.53
1:F:1303:GLY:O	1:F:1306:ALA:N	2.41	0.53
1:B:26:VAL:N	2:H:1889:VAL:O	2.68	0.53
2:I:1971:GLY:C	2:I:1972:ILE:HA	2.29	0.52
2:H:770:GLY:HA2	2:H:1059:ALA:HB2	1.93	0.51
2:L:770:GLY:HA2	2:L:1059:ALA:HB2	1.93	0.51
2:J:770:GLY:HA2	2:J:1059:ALA:HB2	1.93	0.51
2:G:770:GLY:HA2	2:G:1059:ALA:HB2	1.93	0.51
2:I:770:GLY:HA2	2:I:1059:ALA:HB2	1.93	0.51
1:D:1405:ALA:HB1	1:D:1525:ALA:HB1	1.94	0.50
1:D:1303:GLY:O	1:D:1305:CYS:N	2.45	0.50
1:E:1303:GLY:O	1:E:1305:CYS:N	2.45	0.50
1:E:1405:ALA:HB1	1:E:1525:ALA:HB1	1.94	0.50
1:F:1405:ALA:HB1	1:F:1525:ALA:HB1	1.95	0.50
1:A:1303:GLY:O	1:A:1305:CYS:N	2.45	0.49
1:F:1303:GLY:O	1:F:1305:CYS:N	2.45	0.49
1:A:1405:ALA:HB1	1:A:1525:ALA:HB1	1.94	0.49
1:C:1405:ALA:HB1	1:C:1525:ALA:HB1	1.94	0.49
1:D:1584:PRO:O	1:D:1586:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:SER:O	1:A:881:ASN:N	2.46	0.49
1:C:1584:PRO:O	1:C:1586:GLY:N	2.46	0.49
1:C:879:SER:O	1:C:881:ASN:N	2.45	0.49
1:F:1576:PHE:O	1:F:1578:LYS:N	2.46	0.49
1:F:879:SER:O	1:F:881:ASN:N	2.46	0.49
1:A:1576:PHE:O	1:A:1578:LYS:N	2.46	0.49
1:B:1584:PRO:O	1:B:1586:GLY:N	2.46	0.49
1:B:879:SER:O	1:B:881:ASN:N	2.46	0.49
1:E:879:SER:O	1:E:881:ASN:N	2.46	0.49
1:D:879:SER:O	1:D:881:ASN:N	2.46	0.49
1:E:1576:PHE:O	1:E:1578:LYS:N	2.46	0.49
1:F:1584:PRO:O	1:F:1586:GLY:N	2.46	0.49
2:K:770:GLY:HA2	2:K:1059:ALA:HB2	1.93	0.49
1:D:1576:PHE:O	1:D:1578:LYS:N	2.46	0.49
1:B:1405:ALA:HB1	1:B:1525:ALA:HB1	1.94	0.49
1:B:1430:ARG:HA	1:D:1716:LEU:HA	2.29	0.49
1:C:1303:GLY:O	1:C:1305:CYS:N	2.45	0.49
1:E:1584:PRO:O	1:E:1586:GLY:N	2.46	0.49
1:F:26:VAL:N	2:L:1889:VAL:O	2.66	0.49
1:C:1576:PHE:O	1:C:1578:LYS:N	2.46	0.49
1:B:1303:GLY:O	1:B:1305:CYS:N	2.45	0.48
1:B:1576:PHE:O	1:B:1578:LYS:N	2.46	0.48
1:A:1584:PRO:O	1:A:1586:GLY:N	2.46	0.48
1:D:180:SER:O	1:D:183:GLN:N	2.45	0.48
2:I:300:ILE:O	2:I:303:LEU:N	2.47	0.48
2:J:300:ILE:O	2:J:303:LEU:N	2.47	0.48
2:K:300:ILE:O	2:K:303:LEU:N	2.47	0.48
1:E:184:ASN:O	1:E:188:GLY:N	2.66	0.48
2:H:300:ILE:O	2:H:303:LEU:N	2.47	0.48
2:G:300:ILE:O	2:G:303:LEU:N	2.47	0.47
2:L:300:ILE:O	2:L:303:LEU:N	2.47	0.47
2:G:1867:SER:O	2:G:1870:ALA:HB3	2.15	0.47
2:H:1867:SER:O	2:H:1870:ALA:HB3	2.15	0.47
2:I:1867:SER:O	2:I:1870:ALA:HB3	2.15	0.47
2:K:1867:SER:O	2:K:1870:ALA:HB3	2.15	0.46
2:J:1867:SER:O	2:J:1870:ALA:HB3	2.16	0.46
1:E:47:ILE:O	2:K:1666:PHE:HA	2.46	0.46
2:L:1867:SER:O	2:L:1870:ALA:HB3	2.16	0.46
1:F:29:ILE:N	2:L:1891:TYR:O	2.61	0.45
1:E:1023:GLY:O	1:E:1386:ILE:N	2.48	0.45
1:B:1023:GLY:O	1:B:1386:ILE:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1356:GLY:HA2	2:L:1609:THR:HA	1.99	0.45
2:J:1356:GLY:HA2	2:J:1609:THR:HA	1.99	0.45
2:K:1356:GLY:HA2	2:K:1609:THR:HA	1.99	0.44
1:A:1023:GLY:O	1:A:1386:ILE:N	2.48	0.44
1:C:1023:GLY:O	1:C:1386:ILE:N	2.48	0.44
1:F:1023:GLY:O	1:F:1386:ILE:N	2.48	0.44
1:B:1121:MET:O	1:B:1177:LYS:N	2.46	0.44
1:C:357:GLY:HA3	1:D:357:GLY:HA3	3.20	0.44
2:I:1356:GLY:HA2	2:I:1609:THR:HA	1.99	0.44
2:K:317:THR:HA	2:L:1307:ASN:O	2.18	0.44
2:H:1356:GLY:HA2	2:H:1609:THR:HA	1.99	0.44
2:G:1356:GLY:HA2	2:G:1609:THR:HA	1.99	0.43
1:C:181:THR:CB	2:H:510:SER:CA	4.76	0.43
1:F:1121:MET:O	1:F:1177:LYS:N	2.46	0.43
1:F:180:SER:O	1:F:183:GLN:C	2.53	0.43
1:E:1121:MET:O	1:E:1177:LYS:N	2.46	0.43
1:E:46:GLU:HA	2:K:1665:VAL:O	2.47	0.43
2:K:2015:THR:O	2:K:2017:LYS:N	2.46	0.43
1:D:1023:GLY:O	1:D:1386:ILE:N	2.48	0.42
1:C:1121:MET:O	1:C:1177:LYS:N	2.45	0.42
1:A:1121:MET:O	1:A:1177:LYS:N	2.46	0.42
1:A:44:VAL:HA	2:G:1663:THR:O	2.20	0.42
1:F:180:SER:O	1:F:183:GLN:N	2.53	0.42
1:B:1301:PRO:HA	1:D:1300:THR:O	2.45	0.42
2:J:2015:THR:O	2:J:2017:LYS:N	2.46	0.42
1:B:870:GLY:HA3	1:B:927:ASN:HA	2.02	0.42
2:L:1373:SER:O	2:L:1397:SER:N	2.51	0.41
1:C:870:GLY:HA3	1:C:927:ASN:HA	2.03	0.41
1:E:870:GLY:HA3	1:E:927:ASN:HA	2.03	0.41
1:F:666:ALA:O	1:F:670:GLY:HA2	2.21	0.41
1:B:666:ALA:O	1:B:670:GLY:HA2	2.21	0.41
1:D:184:ASN:O	1:D:188:GLY:N	2.65	0.41
2:J:1373:SER:O	2:J:1397:SER:N	2.51	0.41
1:A:870:GLY:HA3	1:A:927:ASN:HA	2.03	0.41
1:C:180:SER:HA	1:C:183:GLN:CB	2.51	0.41
2:G:2015:THR:O	2:G:2017:LYS:N	2.46	0.41
1:A:666:ALA:O	1:A:670:GLY:HA2	2.21	0.41
1:D:666:ALA:O	1:D:670:GLY:HA2	2.21	0.41
2:K:1373:SER:O	2:K:1397:SER:N	2.51	0.41
1:F:870:GLY:HA3	1:F:927:ASN:HA	2.02	0.41
2:H:1373:SER:O	2:H:1397:SER:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:666:ALA:O	1:E:670:GLY:HA2	2.21	0.40
2:K:898:ASP:O	2:K:1050:ARG:HA	2.22	0.40
1:C:666:ALA:O	1:C:670:GLY:HA2	2.21	0.40
2:G:1373:SER:O	2:G:1397:SER:N	2.51	0.40
2:I:1373:SER:O	2:I:1397:SER:N	2.51	0.40
2:L:898:ASP:O	2:L:1050:ARG:HA	2.22	0.40

All (4) 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)
2:G:1929:LYS:CB	2:h:1399:ASN:O[2_645]	1.63	0.57
2:I:1929:LYS:O	2:j:444:VAL:CB[1_655]	1.72	0.48
2:I:1929:LYS:O	2:j:444:VAL:CA[1_655]	2.16	0.04
2:I:1929:LYS:C	2:j:444:VAL:CB[1_655]	2.17	0.03

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	1752/1887 (93%)	1652 (94%)	96 (6%)	4 (0%)	47	81
1	B	1752/1887 (93%)	1647 (94%)	101 (6%)	4 (0%)	47	81
1	C	1752/1887 (93%)	1651 (94%)	97 (6%)	4 (0%)	47	81
1	D	1752/1887 (93%)	1652 (94%)	96 (6%)	4 (0%)	47	81
1	E	1752/1887 (93%)	1649 (94%)	98 (6%)	5 (0%)	41	76
1	F	1752/1887 (93%)	1649 (94%)	98 (6%)	5 (0%)	41	76
1	a	1752/1887 (93%)	1647 (94%)	99 (6%)	6 (0%)	41	76
1	b	1752/1887 (93%)	1649 (94%)	99 (6%)	4 (0%)	47	81
1	c	1752/1887 (93%)	1649 (94%)	98 (6%)	5 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	1752/1887 (93%)	1652 (94%)	96 (6%)	4 (0%)	47	81
1	e	1752/1887 (93%)	1650 (94%)	97 (6%)	5 (0%)	41	76
1	f	1752/1887 (93%)	1649 (94%)	99 (6%)	4 (0%)	47	81
2	G	2029/2051 (99%)	1901 (94%)	120 (6%)	8 (0%)	34	72
2	H	2029/2051 (99%)	1900 (94%)	121 (6%)	8 (0%)	34	72
2	I	2027/2051 (99%)	1902 (94%)	117 (6%)	8 (0%)	34	72
2	J	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	34	72
2	K	2029/2051 (99%)	1903 (94%)	118 (6%)	8 (0%)	34	72
2	L	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	34	72
2	g	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	34	72
2	h	2029/2051 (99%)	1900 (94%)	121 (6%)	8 (0%)	34	72
2	i	2029/2051 (99%)	1903 (94%)	118 (6%)	8 (0%)	34	72
2	j	2029/2051 (99%)	1902 (94%)	119 (6%)	8 (0%)	34	72
2	k	2029/2051 (99%)	1901 (94%)	120 (6%)	8 (0%)	34	72
2	l	2029/2051 (99%)	1903 (94%)	118 (6%)	8 (0%)	34	72
3	M	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	N	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	O	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	P	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	Q	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	R	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	m	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	n	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	o	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	p	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	q	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
3	r	107/150 (71%)	98 (92%)	8 (8%)	1 (1%)	17	56
All	All	46654/49056 (95%)	43793 (94%)	2699 (6%)	162 (0%)	41	76

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1304	ALA

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Mol	Chain	Res	Type
1	B	1304	ALA
1	C	1304	ALA
1	D	1304	ALA
1	E	179	LYS
1	E	1304	ALA
1	F	179	LYS
1	F	1304	ALA
2	G	274	SER
2	G	1317	ARG
2	G	1808	SER
2	H	274	SER
2	H	1317	ARG
2	H	1808	SER
2	I	274	SER
2	I	1317	ARG
2	I	1808	SER
2	J	274	SER
2	J	1317	ARG
2	J	1808	SER
2	K	274	SER
2	K	1317	ARG
2	K	1808	SER
2	L	274	SER
2	L	1317	ARG
2	L	1808	SER
1	a	1304	ALA
1	b	1304	ALA
1	c	179	LYS
1	c	1304	ALA
1	d	1304	ALA
1	e	179	LYS
1	e	1304	ALA
1	f	1304	ALA
2	g	274	SER
2	g	1317	ARG
2	g	1808	SER
2	h	274	SER
2	h	1317	ARG
2	h	1808	SER
2	i	274	SER
2	i	1317	ARG
2	i	1808	SER

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Mol	Chain	Res	Type
2	j	274	SER
2	j	1317	ARG
2	j	1808	SER
2	k	274	SER
2	k	1317	ARG
2	k	1808	SER
2	l	274	SER
2	l	1317	ARG
2	l	1808	SER
1	A	880	ALA
1	A	1577	GLN
1	B	880	ALA
1	B	1577	GLN
1	C	880	ALA
1	C	1577	GLN
1	D	880	ALA
1	D	1577	GLN
1	E	880	ALA
1	E	1577	GLN
1	F	880	ALA
1	F	1577	GLN
2	H	1846	GLU
2	J	1846	GLU
2	K	1846	GLU
2	L	1846	GLU
3	M	148	ILE
3	N	148	ILE
3	O	148	ILE
3	P	148	ILE
3	Q	148	ILE
3	R	148	ILE
1	a	183	GLN
1	a	880	ALA
1	a	1577	GLN
1	b	880	ALA
1	b	1577	GLN
1	c	880	ALA
1	c	1577	GLN
1	d	880	ALA
1	d	1577	GLN
1	e	880	ALA
1	e	1577	GLN

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Mol	Chain	Res	Type
1	f	880	ALA
1	f	1577	GLN
2	g	1846	GLU
2	h	1846	GLU
2	i	1846	GLU
2	j	1846	GLU
2	k	1846	GLU
2	l	1846	GLU
3	m	148	ILE
3	n	148	ILE
3	o	148	ILE
3	p	148	ILE
3	q	148	ILE
3	r	148	ILE
1	A	1585	LYS
1	B	1585	LYS
1	C	1585	LYS
1	D	1585	LYS
1	E	1585	LYS
2	G	1846	GLU
2	G	2016	ALA
2	H	2016	ALA
2	I	1846	GLU
2	I	2016	ALA
2	J	2016	ALA
2	K	2016	ALA
2	L	2016	ALA
1	a	1585	LYS
1	b	1585	LYS
1	c	1585	LYS
1	d	1585	LYS
1	e	1585	LYS
1	f	1585	LYS
2	g	2016	ALA
2	h	2016	ALA
2	i	2016	ALA
2	j	2016	ALA
2	k	2016	ALA
2	l	2016	ALA
1	F	1585	LYS
2	G	1316	ASP
2	H	1316	ASP

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Mol	Chain	Res	Type
2	I	1316	ASP
2	J	1316	ASP
2	K	1316	ASP
2	L	1316	ASP
2	g	1316	ASP
2	h	1316	ASP
2	i	1316	ASP
2	i	1869	GLU
2	j	1316	ASP
2	k	1316	ASP
2	l	1316	ASP
2	G	1214	LEU
2	G	1869	GLU
2	H	1869	GLU
2	I	1869	GLU
2	J	1869	GLU
2	K	1869	GLU
2	L	1869	GLU
2	g	1869	GLU
2	h	1869	GLU
2	j	1869	GLU
2	k	1214	LEU
2	l	1869	GLU
2	H	1214	LEU
2	I	1214	LEU
2	J	1214	LEU
2	K	1214	LEU
2	L	1214	LEU
2	g	1214	LEU
2	h	1214	LEU
2	i	1214	LEU
2	j	1214	LEU
2	k	1869	GLU
2	l	1214	LEU
1	a	182	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	3
2	G	2
2	j	2
2	i	2
2	K	2
2	g	2
2	H	2
2	l	2
2	J	2
2	h	2
2	L	2
2	k	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	299:ALA	C	300:ILE	N	4.56
1	I	299:ALA	C	300:ILE	N	4.56
1	i	299:ALA	C	300:ILE	N	4.56
1	j	299:ALA	C	300:ILE	N	4.56
1	H	299:ALA	C	300:ILE	N	4.55
1	J	299:ALA	C	300:ILE	N	4.55
1	K	299:ALA	C	300:ILE	N	4.55
1	L	299:ALA	C	300:ILE	N	4.55
1	g	299:ALA	C	300:ILE	N	4.55
1	h	299:ALA	C	300:ILE	N	4.55
1	k	299:ALA	C	300:ILE	N	4.55
1	l	299:ALA	C	300:ILE	N	4.55
1	H	300:ILE	C	301:THR	N	3.90
1	K	300:ILE	C	301:THR	N	3.90
1	h	300:ILE	C	301:THR	N	3.90
1	i	300:ILE	C	301:THR	N	3.90
1	k	300:ILE	C	301:THR	N	3.90
1	G	300:ILE	C	301:THR	N	3.89
1	I	300:ILE	C	301:THR	N	3.89
1	J	300:ILE	C	301:THR	N	3.89
1	L	300:ILE	C	301:THR	N	3.89
1	g	300:ILE	C	301:THR	N	3.89
1	j	300:ILE	C	301:THR	N	3.89
1	l	300:ILE	C	301:THR	N	3.89
1	I	1971:GLY	C	1972:ILE	N	2.00

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.