Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2022 – 02:06 PM EDT

PDB ID	:	3WKR
Title	:	Crystal structure of the SepCysS-SepCysE complex from Methanocaldococcus jannaschii
Authors	:	Nakazawa, Y.; Asano, N.; Nakamura, A.; Yao, M.
Deposited on	:	2013-10-30
Resolution	:	2.80 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 (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:

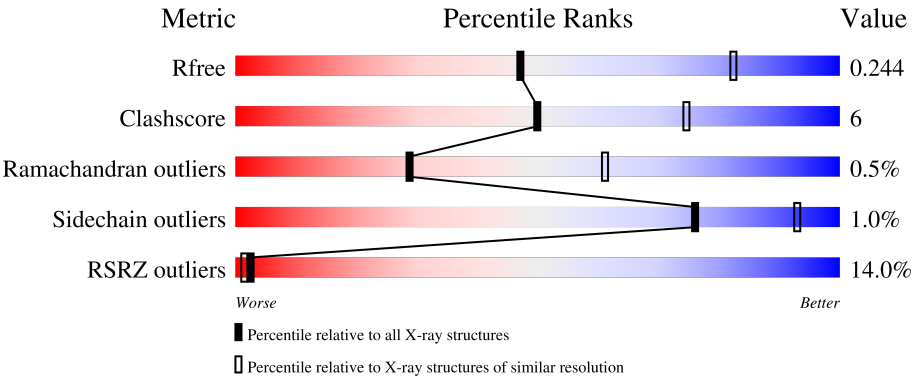
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	416	9% 73% 13% 13%
1	B	416	9% 72% 15% · 12%
1	E	416	14% 71% 16% 12%
1	F	416	18% 71% 16% 13%
2	C	216	% 27% · 69%

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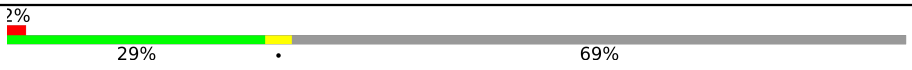
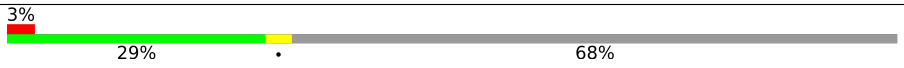
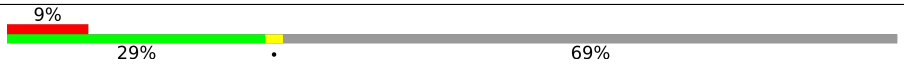
Mol	Chain	Length	Quality of chain
2	D	216	
2	G	216	
2	H	216	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14030 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 O-phospho-L-seryl-tRNA:Cys-tRNA synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	P	S	0	0	0
			2903	1865	485	539	1	13			
1	B	364	Total	C	N	O	P	S	0	0	0
			2916	1873	487	541	1	14			
1	E	365	Total	C	N	O	P	S	0	0	0
			2923	1877	488	543	1	14			
1	F	363	Total	C	N	O	P	S	0	0	0
			2910	1870	486	540	1	13			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q59072
A	-18	GLY	-	expression tag	UNP Q59072
A	-17	SER	-	expression tag	UNP Q59072
A	-16	SER	-	expression tag	UNP Q59072
A	-15	HIS	-	expression tag	UNP Q59072
A	-14	HIS	-	expression tag	UNP Q59072
A	-13	HIS	-	expression tag	UNP Q59072
A	-12	HIS	-	expression tag	UNP Q59072
A	-11	HIS	-	expression tag	UNP Q59072
A	-10	HIS	-	expression tag	UNP Q59072
A	-9	SER	-	expression tag	UNP Q59072
A	-8	SER	-	expression tag	UNP Q59072
A	-7	GLY	-	expression tag	UNP Q59072
A	-6	LEU	-	expression tag	UNP Q59072
A	-5	VAL	-	expression tag	UNP Q59072
A	-4	PRO	-	expression tag	UNP Q59072
A	-3	ARG	-	expression tag	UNP Q59072
A	-2	GLY	-	expression tag	UNP Q59072
A	-1	SER	-	expression tag	UNP Q59072
A	0	HIS	-	expression tag	UNP Q59072
A	1	MET	-	expression tag	UNP Q59072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	-	expression tag	UNP Q59072
A	3	LEU	-	expression tag	UNP Q59072
A	4	GLU	-	expression tag	UNP Q59072
A	5	GLY	-	expression tag	UNP Q59072
A	6	PRO	-	expression tag	UNP Q59072
A	7	TYR	-	expression tag	UNP Q59072
A	8	SER	-	expression tag	UNP Q59072
A	9	LYS	-	expression tag	UNP Q59072
A	10	LYS	-	expression tag	UNP Q59072
A	11	PHE	-	expression tag	UNP Q59072
A	12	GLU	-	expression tag	UNP Q59072
A	13	VAL	-	expression tag	UNP Q59072
A	14	ILE	-	expression tag	UNP Q59072
A	15	THR	-	expression tag	UNP Q59072
A	16	LEU	-	expression tag	UNP Q59072
A	17	ASP	-	expression tag	UNP Q59072
A	18	ILE	-	expression tag	UNP Q59072
A	19	ASN	-	expression tag	UNP Q59072
A	20	LEU	-	expression tag	UNP Q59072
B	-19	MET	-	expression tag	UNP Q59072
B	-18	GLY	-	expression tag	UNP Q59072
B	-17	SER	-	expression tag	UNP Q59072
B	-16	SER	-	expression tag	UNP Q59072
B	-15	HIS	-	expression tag	UNP Q59072
B	-14	HIS	-	expression tag	UNP Q59072
B	-13	HIS	-	expression tag	UNP Q59072
B	-12	HIS	-	expression tag	UNP Q59072
B	-11	HIS	-	expression tag	UNP Q59072
B	-10	HIS	-	expression tag	UNP Q59072
B	-9	SER	-	expression tag	UNP Q59072
B	-8	SER	-	expression tag	UNP Q59072
B	-7	GLY	-	expression tag	UNP Q59072
B	-6	LEU	-	expression tag	UNP Q59072
B	-5	VAL	-	expression tag	UNP Q59072
B	-4	PRO	-	expression tag	UNP Q59072
B	-3	ARG	-	expression tag	UNP Q59072
B	-2	GLY	-	expression tag	UNP Q59072
B	-1	SER	-	expression tag	UNP Q59072
B	0	HIS	-	expression tag	UNP Q59072
B	1	MET	-	expression tag	UNP Q59072
B	2	GLU	-	expression tag	UNP Q59072
B	3	LEU	-	expression tag	UNP Q59072

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLU	-	expression tag	UNP Q59072
B	5	GLY	-	expression tag	UNP Q59072
B	6	PRO	-	expression tag	UNP Q59072
B	7	TYR	-	expression tag	UNP Q59072
B	8	SER	-	expression tag	UNP Q59072
B	9	LYS	-	expression tag	UNP Q59072
B	10	LYS	-	expression tag	UNP Q59072
B	11	PHE	-	expression tag	UNP Q59072
B	12	GLU	-	expression tag	UNP Q59072
B	13	VAL	-	expression tag	UNP Q59072
B	14	ILE	-	expression tag	UNP Q59072
B	15	THR	-	expression tag	UNP Q59072
B	16	LEU	-	expression tag	UNP Q59072
B	17	ASP	-	expression tag	UNP Q59072
B	18	ILE	-	expression tag	UNP Q59072
B	19	ASN	-	expression tag	UNP Q59072
B	20	LEU	-	expression tag	UNP Q59072
E	-19	MET	-	expression tag	UNP Q59072
E	-18	GLY	-	expression tag	UNP Q59072
E	-17	SER	-	expression tag	UNP Q59072
E	-16	SER	-	expression tag	UNP Q59072
E	-15	HIS	-	expression tag	UNP Q59072
E	-14	HIS	-	expression tag	UNP Q59072
E	-13	HIS	-	expression tag	UNP Q59072
E	-12	HIS	-	expression tag	UNP Q59072
E	-11	HIS	-	expression tag	UNP Q59072
E	-10	HIS	-	expression tag	UNP Q59072
E	-9	SER	-	expression tag	UNP Q59072
E	-8	SER	-	expression tag	UNP Q59072
E	-7	GLY	-	expression tag	UNP Q59072
E	-6	LEU	-	expression tag	UNP Q59072
E	-5	VAL	-	expression tag	UNP Q59072
E	-4	PRO	-	expression tag	UNP Q59072
E	-3	ARG	-	expression tag	UNP Q59072
E	-2	GLY	-	expression tag	UNP Q59072
E	-1	SER	-	expression tag	UNP Q59072
E	0	HIS	-	expression tag	UNP Q59072
E	1	MET	-	expression tag	UNP Q59072
E	2	GLU	-	expression tag	UNP Q59072
E	3	LEU	-	expression tag	UNP Q59072
E	4	GLU	-	expression tag	UNP Q59072
E	5	GLY	-	expression tag	UNP Q59072

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	PRO	-	expression tag	UNP Q59072
E	7	TYR	-	expression tag	UNP Q59072
E	8	SER	-	expression tag	UNP Q59072
E	9	LYS	-	expression tag	UNP Q59072
E	10	LYS	-	expression tag	UNP Q59072
E	11	PHE	-	expression tag	UNP Q59072
E	12	GLU	-	expression tag	UNP Q59072
E	13	VAL	-	expression tag	UNP Q59072
E	14	ILE	-	expression tag	UNP Q59072
E	15	THR	-	expression tag	UNP Q59072
E	16	LEU	-	expression tag	UNP Q59072
E	17	ASP	-	expression tag	UNP Q59072
E	18	ILE	-	expression tag	UNP Q59072
E	19	ASN	-	expression tag	UNP Q59072
E	20	LEU	-	expression tag	UNP Q59072
F	-19	MET	-	expression tag	UNP Q59072
F	-18	GLY	-	expression tag	UNP Q59072
F	-17	SER	-	expression tag	UNP Q59072
F	-16	SER	-	expression tag	UNP Q59072
F	-15	HIS	-	expression tag	UNP Q59072
F	-14	HIS	-	expression tag	UNP Q59072
F	-13	HIS	-	expression tag	UNP Q59072
F	-12	HIS	-	expression tag	UNP Q59072
F	-11	HIS	-	expression tag	UNP Q59072
F	-10	HIS	-	expression tag	UNP Q59072
F	-9	SER	-	expression tag	UNP Q59072
F	-8	SER	-	expression tag	UNP Q59072
F	-7	GLY	-	expression tag	UNP Q59072
F	-6	LEU	-	expression tag	UNP Q59072
F	-5	VAL	-	expression tag	UNP Q59072
F	-4	PRO	-	expression tag	UNP Q59072
F	-3	ARG	-	expression tag	UNP Q59072
F	-2	GLY	-	expression tag	UNP Q59072
F	-1	SER	-	expression tag	UNP Q59072
F	0	HIS	-	expression tag	UNP Q59072
F	1	MET	-	expression tag	UNP Q59072
F	2	GLU	-	expression tag	UNP Q59072
F	3	LEU	-	expression tag	UNP Q59072
F	4	GLU	-	expression tag	UNP Q59072
F	5	GLY	-	expression tag	UNP Q59072
F	6	PRO	-	expression tag	UNP Q59072
F	7	TYR	-	expression tag	UNP Q59072

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Chain	Residue	Modelled	Actual	Comment	Reference
F	8	SER	-	expression tag	UNP Q59072
F	9	LYS	-	expression tag	UNP Q59072
F	10	LYS	-	expression tag	UNP Q59072
F	11	PHE	-	expression tag	UNP Q59072
F	12	GLU	-	expression tag	UNP Q59072
F	13	VAL	-	expression tag	UNP Q59072
F	14	ILE	-	expression tag	UNP Q59072
F	15	THR	-	expression tag	UNP Q59072
F	16	LEU	-	expression tag	UNP Q59072
F	17	ASP	-	expression tag	UNP Q59072
F	18	ILE	-	expression tag	UNP Q59072
F	19	ASN	-	expression tag	UNP Q59072
F	20	LEU	-	expression tag	UNP Q59072

- Molecule 2 is a protein called Uncharacterized protein MJ1481.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	68	Total	C	N	O	S	0	0	0
			562	368	89	103	2			
2	D	68	Total	C	N	O	S	0	0	0
			565	371	89	103	2			
2	G	69	Total	C	N	O	S	0	0	0
			573	377	90	104	2			
2	H	68	Total	C	N	O	S	0	0	0
			565	371	89	103	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	MET	-	expression tag	UNP Q58876
C	-1	ASN	-	expression tag	UNP Q58876
C	0	HIS	-	expression tag	UNP Q58876
D	-2	MET	-	expression tag	UNP Q58876
D	-1	ASN	-	expression tag	UNP Q58876
D	0	HIS	-	expression tag	UNP Q58876
G	-2	MET	-	expression tag	UNP Q58876
G	-1	ASN	-	expression tag	UNP Q58876
G	0	HIS	-	expression tag	UNP Q58876
H	-2	MET	-	expression tag	UNP Q58876
H	-1	ASN	-	expression tag	UNP Q58876
H	0	HIS	-	expression tag	UNP Q58876

- Molecule 3 is water.

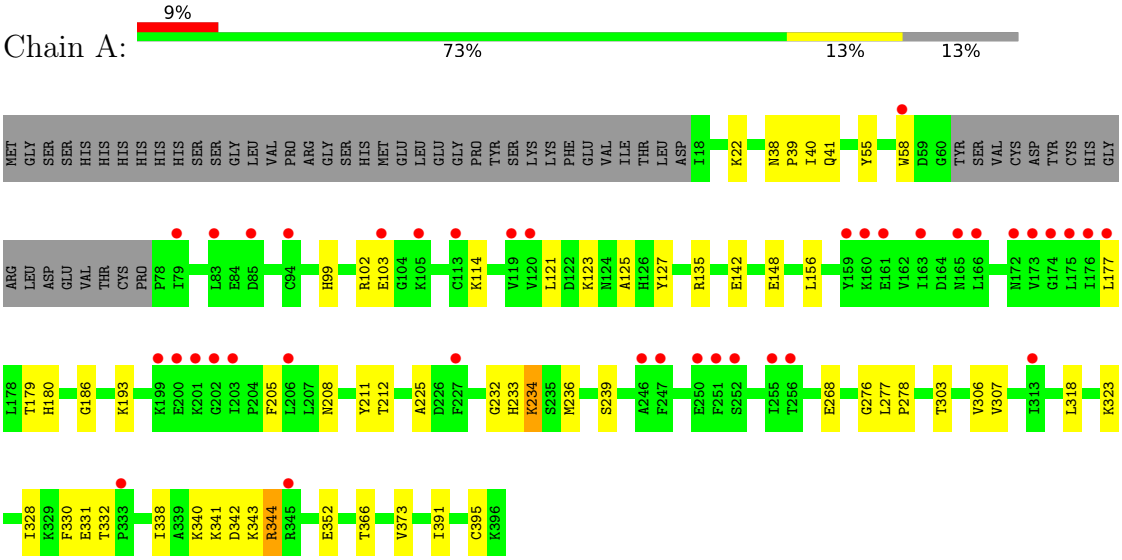
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	26	Total O 26 26	0	0
3	C	4	Total O 4 4	0	0
3	D	4	Total O 4 4	0	0
3	E	22	Total O 22 22	0	0
3	F	20	Total O 20 20	0	0
3	G	6	Total O 6 6	0	0
3	H	7	Total O 7 7	0	0

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.

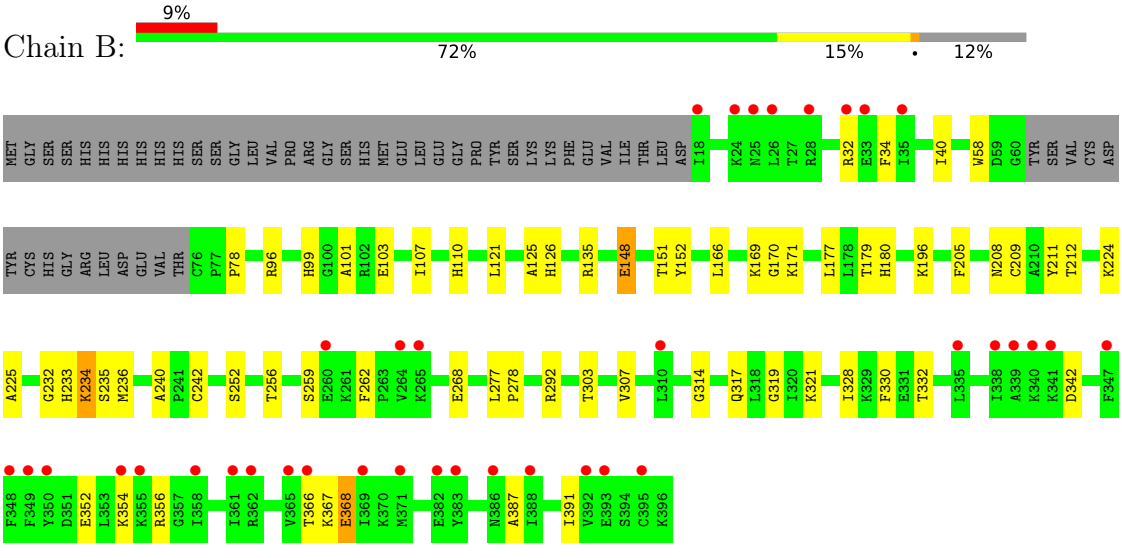
• Molecule 1: O-phospho-L-seryl-tRNA:Cys-tRNA synthase

Chain A:



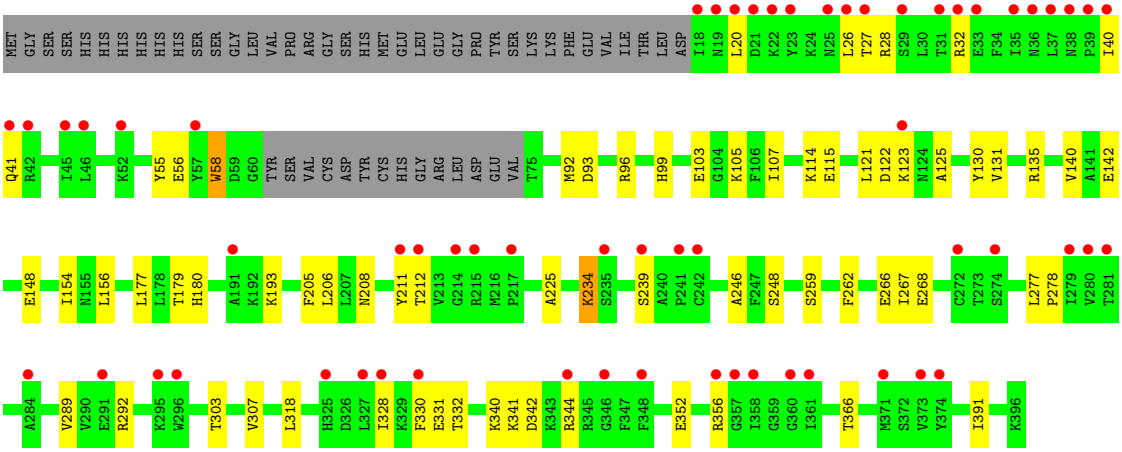
• Molecule 1: O-phospho-L-seryl-tRNA:Cys-tRNA synthase

Chain B:



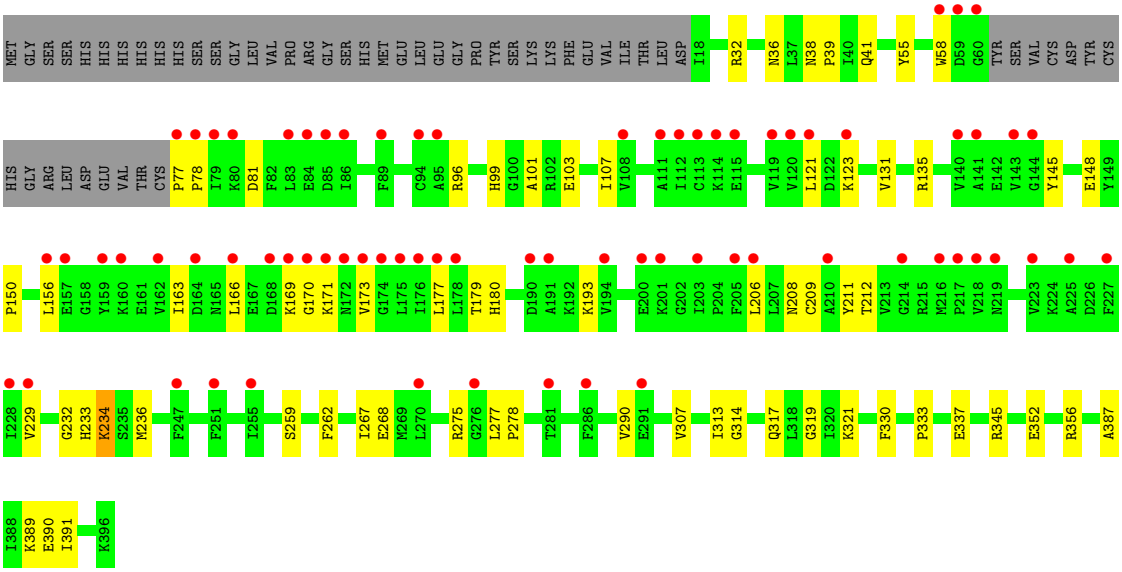
• Molecule 1: O-phospho-L-seryl-tRNA:Cys-tRNA synthase

Chain E:



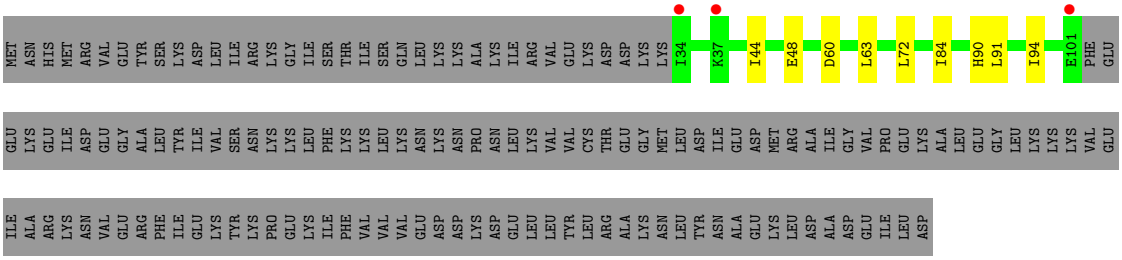
• Molecule 1: O-phospho-L-seryl-tRNA:Cys-tRNA synthase

Chain F:



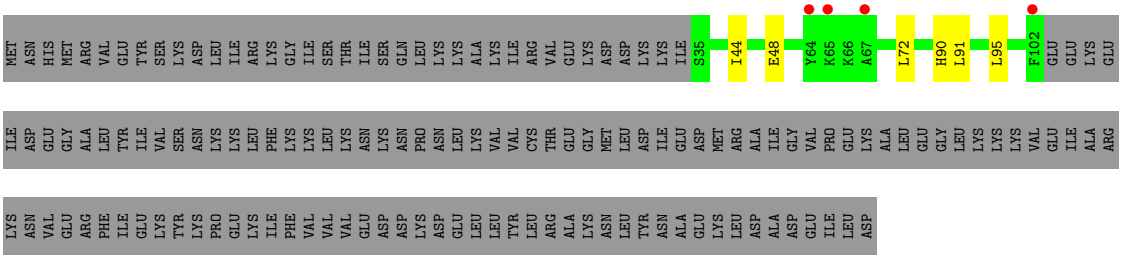
• Molecule 2: Uncharacterized protein MJ1481

Chain C:

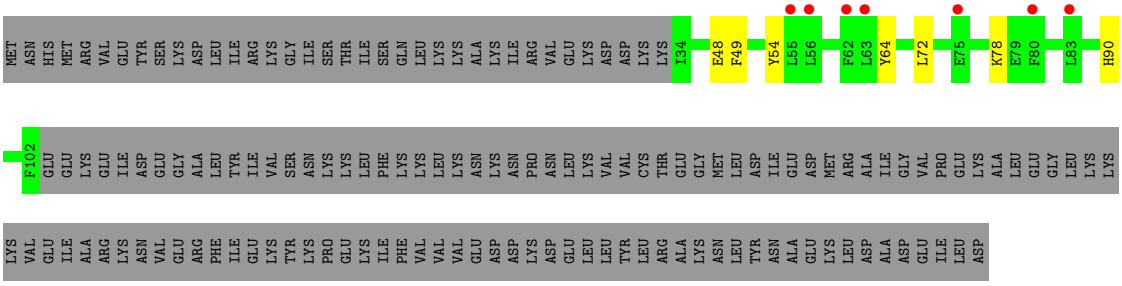


• Molecule 2: Uncharacterized protein MJ1481

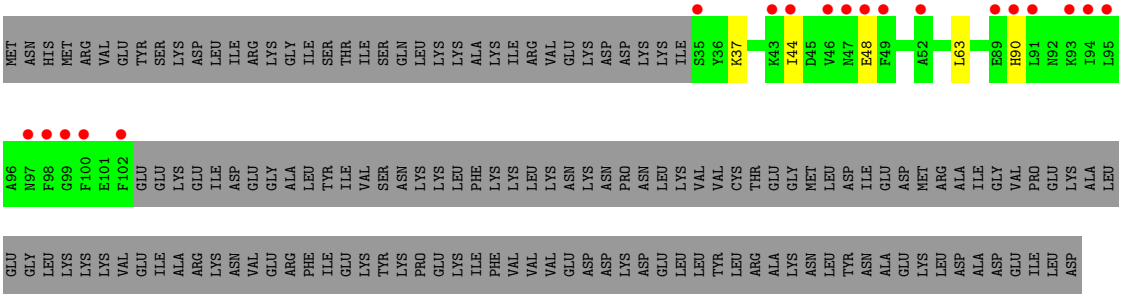
Chain D:



• Molecule 2: Uncharacterized protein MJ1481



• Molecule 2: Uncharacterized protein MJ1481



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	106.88Å 106.88Å 495.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.30 – 2.80 47.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (47.30-2.80) 94.9 (47.30-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.224 , 0.242 0.228 , 0.244	Depositor DCC
R_{free} test set	4279 reflections (5.78%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.467 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.498 for h,-h-k,-l	Depositor
Outliers	0 of 74017 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14030	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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

5.1 Standard geometry

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

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	0.20	0/2933	0.35	0/3939
1	B	0.21	0/2947	0.36	0/3960
1	E	0.20	0/2954	0.36	0/3970
1	F	0.21	0/2941	0.35	0/3951
2	C	0.21	0/573	0.31	0/765
2	D	0.21	0/577	0.30	0/770
2	G	0.21	0/585	0.30	0/781
2	H	0.21	0/577	0.30	0/770
All	All	0.21	0/14087	0.35	0/18906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2903	0	2951	35	0
1	B	2916	0	2962	44	0
1	E	2923	0	2969	45	0
1	F	2910	0	2958	43	0
2	C	562	0	571	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	565	0	569	5	0
2	G	573	0	580	6	0
2	H	565	0	569	4	0
3	A	24	0	0	0	0
3	B	26	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	22	0	0	0	0
3	F	20	0	0	0	0
3	G	6	0	0	0	0
3	H	7	0	0	0	0
All	All	14030	0	14129	162	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 6.

All (162) 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:B:101:ALA:HB3	1:B:234:LLP:H5'2	1.73	0.71
1:A:268:GLU:HA	1:B:135:ARG:HD2	1.75	0.69
1:B:232:GLY:HA2	1:B:236:MET:HB2	1.75	0.68
1:E:268:GLU:HA	1:F:135:ARG:HD2	1.77	0.66
1:E:55:TYR:O	1:F:32:ARG:NH1	2.26	0.66
1:E:135:ARG:HD2	1:F:268:GLU:HA	1.79	0.65
1:E:107:ILE:HG23	1:E:268:GLU:HG2	1.79	0.65
1:E:234:LLP:NZ	1:E:234:LLP:O3	2.27	0.65
1:A:352:GLU:HB3	1:A:391:ILE:HD12	1.79	0.65
1:A:55:TYR:O	1:B:32:ARG:NH1	2.28	0.64
1:E:340:LYS:HG2	1:E:341:LYS:HG3	1.79	0.63
1:A:318:LEU:HD11	1:A:331:GLU:HB2	1.80	0.63
1:A:99:HIS:HB2	1:A:103:GLU:HG3	1.79	0.63
1:A:232:GLY:HA2	1:A:236:MET:HB2	1.80	0.63
1:B:121:LEU:HB3	1:B:177:LEU:HB3	1.81	0.62
1:F:352:GLU:HB3	1:F:391:ILE:HD12	1.81	0.62
1:A:340:LYS:HG2	1:A:341:LYS:HG3	1.81	0.62
1:B:179:THR:HA	1:B:208:ASN:HB3	1.81	0.62
1:B:234:LLP:O3	1:B:234:LLP:NZ	2.29	0.62
1:B:367:LYS:HG3	1:B:368:GLU:HG2	1.82	0.62
1:E:179:THR:HA	1:E:208:ASN:HB3	1.82	0.61
1:A:233:HIS:NE2	1:A:234:LLP:OP2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HD2	1:B:268:GLU:HA	1.83	0.60
1:A:234:LLP:NZ	1:A:234:LLP:O3	2.33	0.60
1:B:352:GLU:HB3	1:B:391:ILE:HD12	1.82	0.60
1:E:307:VAL:HA	1:E:330:PHE:HZ	1.67	0.60
1:B:242:CYS:HB2	1:B:278:PRO:HB2	1.84	0.59
1:A:40:ILE:HG13	1:A:41:GLN:HG3	1.84	0.59
1:A:179:THR:HA	1:A:208:ASN:HB3	1.84	0.59
1:E:205:PHE:HD2	1:E:225:ALA:HA	1.67	0.58
1:F:234:LLP:O3	1:F:234:LLP:NZ	2.37	0.58
1:E:179:THR:HG22	1:E:208:ASN:HD22	1.70	0.57
1:A:205:PHE:HD2	1:A:225:ALA:HA	1.69	0.57
1:B:169:LYS:N	1:B:170:GLY:HA2	2.18	0.57
1:F:356:ARG:NH2	1:F:390:GLU:OE1	2.38	0.57
1:E:123:LYS:NZ	1:E:142:GLU:OE1	2.38	0.56
1:B:166:LEU:O	1:B:171:LYS:N	2.37	0.56
1:E:105:LYS:HG2	1:E:206:LEU:HD21	1.89	0.55
1:F:101:ALA:HB3	1:F:234:LLP:H5'2	1.89	0.55
1:F:179:THR:HA	1:F:208:ASN:HB3	1.88	0.55
1:A:276:GLY:HA2	1:B:240:ALA:HB3	1.89	0.55
1:F:99:HIS:HB2	1:F:103:GLU:HG3	1.89	0.54
1:E:352:GLU:HB3	1:E:391:ILE:HD12	1.89	0.54
1:A:102:ARG:NH2	1:A:127:TYR:OH	2.35	0.53
1:E:318:LEU:HD11	1:E:331:GLU:HB2	1.89	0.53
1:A:307:VAL:HA	1:A:330:PHE:HZ	1.73	0.53
1:B:233:HIS:NE2	1:B:234:LLP:OP2	2.34	0.53
1:E:93:ASP:HB2	1:E:248:SER:HA	1.90	0.53
1:E:332:THR:OG1	1:E:366:THR:O	2.26	0.52
1:F:313:ILE:HD11	1:F:389:LYS:HG2	1.91	0.52
1:E:26:LEU:HD11	1:F:77:PRO:HG3	1.91	0.52
1:B:107:ILE:HG23	1:B:268:GLU:HG2	1.92	0.52
1:B:99:HIS:HB2	1:B:103:GLU:HG3	1.92	0.52
1:F:78:PRO:HB2	1:F:81:ASP:HB2	1.93	0.51
1:F:150:PRO:O	1:F:319:GLY:N	2.39	0.51
1:E:125:ALA:HA	1:E:179:THR:HG21	1.93	0.51
1:A:125:ALA:HA	1:A:179:THR:HG21	1.92	0.50
1:F:166:LEU:O	1:F:171:LYS:N	2.44	0.50
2:C:72:LEU:HD11	2:D:44:ILE:HD11	1.93	0.50
1:B:40:ILE:HG23	1:B:234:LLP:HE3	1.92	0.50
1:E:156:LEU:HD12	1:E:193:LYS:HD2	1.94	0.50
1:A:114:LYS:HG2	1:F:345:ARG:HH11	1.77	0.49
1:B:107:ILE:HD12	1:B:268:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PHE:HE2	1:B:354:LYS:HA	1.77	0.49
2:G:72:LEU:HD11	2:H:44:ILE:HD11	1.95	0.49
1:E:239:SER:HB2	1:F:277:LEU:HD13	1.95	0.49
2:C:84:ILE:HB	2:D:95:LEU:HD21	1.95	0.48
1:E:99:HIS:HB2	1:E:103:GLU:HG3	1.96	0.48
1:F:232:GLY:HA2	1:F:236:MET:HB2	1.93	0.48
1:F:121:LEU:HB3	1:F:177:LEU:HB3	1.95	0.48
1:B:126:HIS:HB2	1:B:234:LLP:H2'3	1.96	0.48
1:F:169:LYS:N	1:F:170:GLY:HA2	2.28	0.48
1:A:341:LYS:HA	1:A:342:ASP:HA	1.58	0.47
1:B:342:ASP:O	1:E:114:LYS:NZ	2.39	0.47
1:E:56:GLU:OE2	2:G:54:TYR:OH	2.31	0.47
1:A:277:LEU:N	1:A:278:PRO:HD2	2.30	0.47
1:E:32:ARG:NH2	2:G:64:TYR:OH	2.47	0.47
2:H:48:GLU:OE2	2:H:90:HIS:ND1	2.37	0.47
1:B:307:VAL:HA	1:B:330:PHE:HZ	1.79	0.47
1:A:123:LYS:NZ	1:A:142:GLU:OE1	2.48	0.47
1:B:110:HIS:ND1	1:B:268:GLU:OE2	2.48	0.47
1:A:306:VAL:HG21	1:A:373:VAL:HG11	1.97	0.46
2:C:60:ASP:HA	2:C:63:LEU:HD13	1.96	0.46
1:E:259:SER:OG	1:E:262:PHE:O	2.31	0.46
1:A:22:LYS:HB3	1:B:78:PRO:HG3	1.96	0.46
1:A:338:ILE:HG21	1:A:395:CYS:HB3	1.96	0.46
1:B:196:LYS:HD2	1:B:224:LYS:HE3	1.98	0.46
1:A:179:THR:HG22	1:A:208:ASN:HD22	1.81	0.45
1:A:186:GLY:O	1:A:323:LYS:NZ	2.49	0.45
1:B:148:GLU:O	1:B:152:TYR:N	2.37	0.45
1:F:156:LEU:HD12	1:F:193:LYS:HD2	1.98	0.45
1:F:233:HIS:NE2	1:F:234:LLP:OP2	2.43	0.45
1:F:208:ASN:HD22	1:F:229:VAL:HG23	1.82	0.45
1:E:289:VAL:HA	1:E:292:ARG:HG2	1.98	0.45
1:A:156:LEU:HD12	1:A:193:LYS:HD2	1.98	0.45
1:E:356:ARG:HE	1:E:391:ILE:HD11	1.82	0.45
1:E:107:ILE:HD12	1:E:268:GLU:HG3	1.99	0.44
1:F:36:ASN:ND2	1:F:41:GLN:OE1	2.50	0.44
1:B:235:SER:O	1:B:292:ARG:NH2	2.50	0.44
1:F:209:CYS:HB3	1:F:212:THR:HB	2.00	0.44
1:E:96:ARG:NH2	1:E:266:GLU:OE2	2.51	0.44
2:G:48:GLU:OE2	2:G:90:HIS:ND1	2.37	0.44
1:E:277:LEU:N	1:E:278:PRO:HD2	2.33	0.44
1:A:121:LEU:HB3	1:A:177:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:GLU:O	1:E:107:ILE:HG12	2.18	0.43
1:E:180:HIS:ND1	1:E:212:THR:HG21	2.33	0.43
1:F:103:GLU:O	1:F:107:ILE:HG12	2.18	0.43
1:E:40:ILE:HG13	1:E:41:GLN:HG3	1.99	0.43
1:E:32:ARG:NH1	1:F:55:TYR:O	2.48	0.43
1:B:103:GLU:O	1:B:107:ILE:HG12	2.17	0.43
1:B:252:SER:O	1:B:256:THR:OG1	2.25	0.43
2:G:49:PHE:CD2	2:H:63:LEU:HD11	2.53	0.43
1:A:239:SER:HB2	1:B:277:LEU:HD13	1.99	0.43
1:B:356:ARG:HE	1:B:391:ILE:HD11	1.83	0.43
1:E:131:VAL:HG13	1:F:267:ILE:HA	2.01	0.43
1:B:259:SER:OG	1:B:262:PHE:O	2.32	0.43
1:E:177:LEU:HD12	1:E:206:LEU:HD23	2.01	0.43
1:E:267:ILE:HA	1:F:131:VAL:HG13	2.00	0.43
1:F:123:LYS:HD3	1:F:145:TYR:CE2	2.53	0.43
1:A:239:SER:O	1:A:278:PRO:HB3	2.19	0.43
1:B:205:PHE:HD2	1:B:225:ALA:HA	1.84	0.42
1:A:180:HIS:ND1	1:A:212:THR:HG21	2.32	0.42
1:E:122:ASP:HB2	1:E:154:ILE:HG13	2.01	0.42
1:B:317:GLN:NE2	1:B:321:LYS:HG2	2.34	0.42
2:C:91:LEU:HD23	2:C:94:ILE:HD12	2.02	0.42
1:F:107:ILE:HD12	1:F:268:GLU:HG3	2.00	0.42
1:F:307:VAL:HA	1:F:330:PHE:HZ	1.85	0.42
1:F:387:ALA:O	1:F:391:ILE:HG12	2.19	0.42
1:B:151:THR:O	1:B:319:GLY:HA2	2.20	0.42
2:C:84:ILE:HG23	2:D:91:LEU:HD22	2.01	0.42
1:E:58:TRP:HE1	1:F:32:ARG:HH22	1.68	0.42
1:F:38:ASN:HA	1:F:39:PRO:HD3	1.87	0.42
1:B:209:CYS:HB3	1:B:212:THR:HB	2.02	0.42
1:B:387:ALA:O	1:B:391:ILE:HG12	2.19	0.42
1:E:26:LEU:O	1:E:28:ARG:N	2.52	0.42
1:B:180:HIS:ND1	1:B:212:THR:HG21	2.34	0.42
2:C:48:GLU:OE2	2:C:90:HIS:ND1	2.42	0.42
1:E:130:TYR:CE2	1:E:140:VAL:HG11	2.55	0.42
1:E:341:LYS:HA	1:E:342:ASP:HA	1.65	0.42
1:F:180:HIS:ND1	1:F:212:THR:HG21	2.35	0.42
1:F:277:LEU:N	1:F:278:PRO:HD2	2.35	0.42
1:B:169:LYS:H	1:B:170:GLY:HA2	1.83	0.41
1:B:277:LEU:N	1:B:278:PRO:HD2	2.35	0.41
1:A:38:ASN:HA	1:A:39:PRO:HD3	1.89	0.41
1:E:303:THR:HG23	1:E:328:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ALA:HA	1:B:179:THR:HG21	2.02	0.41
1:F:166:LEU:HA	1:F:169:LYS:HD2	2.02	0.41
1:B:303:THR:HG23	1:B:328:ILE:HD11	2.03	0.41
2:C:44:ILE:HD11	2:D:72:LEU:HD11	2.02	0.41
2:D:48:GLU:OE2	2:D:90:HIS:ND1	2.43	0.41
1:A:343:LYS:HB3	1:A:344:ARG:H	1.68	0.41
1:F:177:LEU:HD12	1:F:206:LEU:HD23	2.02	0.41
1:F:333:PRO:O	1:F:337:GLU:HG2	2.20	0.41
2:G:78:LYS:HE3	2:H:37:LYS:HA	2.03	0.41
1:E:92:MET:HG2	1:E:246:ALA:HB1	2.04	0.40
1:F:163:ILE:HG23	1:F:173:VAL:HG21	2.03	0.40
1:F:259:SER:OG	1:F:262:PHE:O	2.37	0.40
1:A:303:THR:HG23	1:A:328:ILE:HD11	2.02	0.40
1:A:332:THR:OG1	1:A:366:THR:O	2.38	0.40
1:E:20:LEU:HD21	1:F:290:VAL:HG11	2.04	0.40
1:B:332:THR:OG1	1:B:366:THR:O	2.39	0.40
1:F:317:GLN:NE2	1:F:321:LYS:HG2	2.36	0.40

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	357/416 (86%)	333 (93%)	23 (6%)	1 (0%)	41	72
1	B	359/416 (86%)	342 (95%)	15 (4%)	2 (1%)	25	56
1	E	360/416 (86%)	335 (93%)	22 (6%)	3 (1%)	19	49
1	F	358/416 (86%)	340 (95%)	16 (4%)	2 (1%)	25	56
2	C	66/216 (31%)	65 (98%)	1 (2%)	0	100	100
2	D	66/216 (31%)	65 (98%)	1 (2%)	0	100	100
2	G	67/216 (31%)	66 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	66/216 (31%)	65 (98%)	1 (2%)	0	100 100
All	All	1699/2528 (67%)	1611 (95%)	80 (5%)	8 (0%)	29 61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	148	GLU
1	E	115	GLU
1	E	148	GLU
1	F	314	GLY
1	A	148	GLU
1	B	148	GLU
1	E	27	THR
1	B	314	GLY

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	309/358 (86%)	306 (99%)	3 (1%)	76 93
1	B	311/358 (87%)	307 (99%)	4 (1%)	69 91
1	E	312/358 (87%)	308 (99%)	4 (1%)	69 91
1	F	310/358 (87%)	306 (99%)	4 (1%)	69 91
2	C	60/195 (31%)	60 (100%)	0	100 100
2	D	60/195 (31%)	60 (100%)	0	100 100
2	G	61/195 (31%)	61 (100%)	0	100 100
2	H	60/195 (31%)	60 (100%)	0	100 100
All	All	1483/2212 (67%)	1468 (99%)	15 (1%)	76 93

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	TRP
1	A	211	TYR
1	A	344	ARG
1	B	58	TRP
1	B	96	ARG
1	B	211	TYR
1	B	368	GLU
1	E	58	TRP
1	E	121	LEU
1	E	211	TYR
1	E	344	ARG
1	F	58	TRP
1	F	96	ARG
1	F	211	TYR
1	F	275	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	208	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	E	234	1	23,24,25	1.70	3 (13%)	25,32,34	1.81	3 (12%)
1	LLP	F	234	1	23,24,25	1.73	3 (13%)	25,32,34	1.68	5 (20%)
1	LLP	B	234	1	23,24,25	1.70	3 (13%)	25,32,34	1.77	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	A	234	1	23,24,25	1.70	3 (13%)	25,32,34	1.69	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	E	234	1	-	7/16/17/19	0/1/1/1
1	LLP	F	234	1	-	7/16/17/19	0/1/1/1
1	LLP	B	234	1	-	7/16/17/19	0/1/1/1
1	LLP	A	234	1	-	7/16/17/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	234	LLP	O3-C3	-5.84	1.23	1.37
1	F	234	LLP	O3-C3	-5.83	1.23	1.37
1	B	234	LLP	O3-C3	-5.81	1.23	1.37
1	A	234	LLP	O3-C3	-5.78	1.23	1.37
1	F	234	LLP	C2-N1	2.52	1.38	1.33
1	A	234	LLP	C2-N1	2.43	1.38	1.33
1	E	234	LLP	C2-N1	2.41	1.38	1.33
1	B	234	LLP	C2-N1	2.35	1.38	1.33
1	F	234	LLP	C4-C4'	2.16	1.50	1.46
1	B	234	LLP	C4-C4'	2.13	1.50	1.46
1	A	234	LLP	C4-C4'	2.12	1.50	1.46
1	E	234	LLP	C4-C4'	2.09	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	234	LLP	OP4-C5'-C5	6.60	121.94	109.35
1	B	234	LLP	OP4-C5'-C5	6.31	121.37	109.35
1	A	234	LLP	OP4-C5'-C5	5.74	120.29	109.35
1	F	234	LLP	OP4-C5'-C5	5.54	119.92	109.35
1	E	234	LLP	C4-C4'-NZ	-3.24	109.45	124.31
1	B	234	LLP	C4-C4'-NZ	-3.19	109.67	124.31
1	F	234	LLP	C4-C4'-NZ	-3.16	109.78	124.31
1	A	234	LLP	C4-C4'-NZ	-3.00	110.51	124.31
1	A	234	LLP	CE-NZ-C4'	-2.81	110.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	234	LLP	CE-NZ-C4'	-2.79	110.35	118.90
1	E	234	LLP	CE-NZ-C4'	-2.75	110.45	118.90
1	B	234	LLP	CE-NZ-C4'	-2.73	110.51	118.90
1	A	234	LLP	C5-C6-N1	-2.16	120.22	123.82
1	B	234	LLP	C5-C6-N1	-2.08	120.35	123.82
1	F	234	LLP	C5-C6-N1	-2.08	120.36	123.82
1	F	234	LLP	OP3-P-OP2	2.00	115.30	107.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	234	LLP	C4-C4'-NZ-CE
1	A	234	LLP	C4-C5-C5'-OP4
1	A	234	LLP	C6-C5-C5'-OP4
1	A	234	LLP	C5'-OP4-P-OP1
1	A	234	LLP	C5'-OP4-P-OP2
1	A	234	LLP	C5'-OP4-P-OP3
1	B	234	LLP	C4-C4'-NZ-CE
1	B	234	LLP	C4-C5-C5'-OP4
1	B	234	LLP	C6-C5-C5'-OP4
1	B	234	LLP	C5'-OP4-P-OP1
1	B	234	LLP	C5'-OP4-P-OP2
1	B	234	LLP	C5'-OP4-P-OP3
1	B	234	LLP	O-C-CA-CB
1	E	234	LLP	C4-C5-C5'-OP4
1	E	234	LLP	C6-C5-C5'-OP4
1	E	234	LLP	C5'-OP4-P-OP1
1	E	234	LLP	C5'-OP4-P-OP2
1	E	234	LLP	C5'-OP4-P-OP3
1	E	234	LLP	C-CA-CB-CG
1	F	234	LLP	C4-C4'-NZ-CE
1	F	234	LLP	C4-C5-C5'-OP4
1	F	234	LLP	C5'-OP4-P-OP1
1	F	234	LLP	C5'-OP4-P-OP2
1	F	234	LLP	C5'-OP4-P-OP3
1	F	234	LLP	O-C-CA-CB
1	E	234	LLP	C4-C4'-NZ-CE
1	F	234	LLP	C6-C5-C5'-OP4
1	A	234	LLP	CD-CE-NZ-C4'

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	234	LLP	1	0
1	F	234	LLP	3	0
1	B	234	LLP	5	0
1	A	234	LLP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	361/416 (86%)	0.77	39 (10%) 5 3	36, 102, 154, 181	0
1	B	363/416 (87%)	0.68	37 (10%) 6 3	39, 74, 168, 203	0
1	E	364/416 (87%)	0.94	60 (16%) 1 1	42, 102, 163, 201	0
1	F	362/416 (87%)	1.16	73 (20%) 1 0	34, 114, 182, 213	0
2	C	68/216 (31%)	0.64	3 (4%) 34 24	43, 79, 146, 173	0
2	D	68/216 (31%)	0.55	4 (5%) 22 14	39, 71, 169, 182	0
2	G	69/216 (31%)	0.67	7 (10%) 7 4	45, 94, 154, 196	0
2	H	68/216 (31%)	1.33	19 (27%) 0 0	35, 116, 178, 193	0
All	All	1723/2528 (68%)	0.87	242 (14%) 2 1	34, 97, 171, 213	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	172	ASN	10.6
1	F	144	GLY	10.5
1	F	173	VAL	9.4
2	H	100	PHE	8.6
1	B	341	LYS	8.2
2	C	34	ILE	8.2
1	F	174	GLY	7.6
1	F	157	GLU	7.4
1	F	156	LEU	7.1
1	E	23	TYR	6.7
1	F	60	GLY	6.7
1	E	20	LEU	6.7
1	E	35	ILE	6.5
1	F	175	LEU	6.4
1	E	242	CYS	6.2
1	F	168	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	E	25	ASN	5.6
1	A	201	LYS	5.5
1	F	84	GLU	5.4
1	B	358	ILE	5.3
2	H	102	PHE	5.3
1	A	166	LEU	5.3
1	F	159	TYR	5.1
2	C	101	GLU	5.1
1	A	227	PHE	5.1
1	B	338	ILE	5.1
1	A	345	ARG	5.0
1	A	203	ILE	5.0
1	F	218	VAL	4.9
1	F	203	ILE	4.9
1	E	18	ILE	4.8
1	E	239	SER	4.7
1	B	365	VAL	4.7
1	F	194	VAL	4.7
2	H	90	HIS	4.6
1	F	79	ILE	4.6
1	F	83	LEU	4.6
1	B	265	LYS	4.5
1	A	251	PHE	4.4
1	F	247	PHE	4.4
1	E	214	GLY	4.4
2	H	98	PHE	4.4
1	A	79	ILE	4.3
1	A	173	VAL	4.3
1	E	295	LYS	4.3
1	F	217	PRO	4.3
1	E	40	ILE	4.2
1	E	371	MET	4.2
1	F	205	PHE	4.2
1	B	392	VAL	4.2
2	H	46	VAL	4.1
1	F	114	LYS	4.1
1	F	223	VAL	4.1
1	F	58	TRP	4.1
2	H	97	ASN	4.1
1	E	41	GLN	4.0
1	F	77	PRO	4.0
1	F	112	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	350	TYR	4.0
1	F	206	LEU	4.0
1	A	252	SER	3.9
1	F	113	CYS	3.9
1	F	141	ALA	3.9
1	F	200	GLU	3.9
1	E	358	ILE	3.9
1	E	361	ILE	3.8
1	E	215	ARG	3.8
1	F	119	VAL	3.8
1	B	28	ARG	3.8
1	F	115	GLU	3.8
1	A	206	LEU	3.8
1	E	39	PRO	3.8
1	E	32	ARG	3.8
1	E	235	SER	3.7
1	E	22	LYS	3.7
1	E	328	ILE	3.7
1	A	246	ALA	3.7
1	E	274	SER	3.7
1	A	120	VAL	3.6
1	F	177	LEU	3.6
1	E	374	TYR	3.6
1	F	95	ALA	3.6
1	F	160	LYS	3.6
1	B	347	PHE	3.6
1	A	202	GLY	3.5
1	E	211	TYR	3.5
1	E	26	LEU	3.5
2	H	89	GLU	3.5
1	F	111	ALA	3.5
1	A	174	GLY	3.4
1	E	36	ASN	3.4
1	E	325	HIS	3.4
1	B	395	CYS	3.4
1	F	227	PHE	3.4
2	H	43	LYS	3.3
1	F	216	MET	3.3
1	B	388	ILE	3.3
2	H	93	LYS	3.3
1	B	348	PHE	3.3
1	A	250	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	225	ALA	3.3
2	H	94	ILE	3.3
2	H	95	LEU	3.2
1	F	166	LEU	3.2
1	B	371	MET	3.2
1	B	335	LEU	3.2
2	G	75	GLU	3.2
1	B	32	ARG	3.1
1	E	241	PRO	3.1
1	A	200	GLU	3.1
1	F	86	ILE	3.1
1	B	264	VAL	3.1
1	A	172	ASN	3.1
1	F	120	VAL	3.1
2	H	99	GLY	3.1
1	E	19	ASN	3.1
1	A	163	ILE	3.1
1	F	286	PHE	3.0
1	E	33	GLU	3.0
1	A	175	LEU	3.0
1	B	355	LYS	3.0
1	F	229	VAL	3.0
1	F	89	PHE	3.0
1	E	272	CYS	3.0
1	B	349	PHE	3.0
1	E	37	LEU	2.9
1	B	24	LYS	2.9
1	E	291	GLU	2.9
1	E	279	ILE	2.9
1	E	46	LEU	2.9
1	E	212	THR	2.9
1	A	255	ILE	2.9
1	F	140	VAL	2.9
1	F	176	ILE	2.8
2	G	63	LEU	2.8
1	B	382	GLU	2.8
1	E	38	ASN	2.8
1	E	29	SER	2.8
1	B	18	ILE	2.8
2	G	80	PHE	2.7
1	A	85	ASP	2.7
1	F	219	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	64	TYR	2.7
1	E	42	ARG	2.6
1	E	360	GLY	2.6
1	A	199	LYS	2.6
1	E	356	ARG	2.6
1	F	255	ILE	2.6
1	F	94	CYS	2.6
1	B	340	LYS	2.6
1	F	123	LYS	2.6
1	F	291	GLU	2.6
1	F	170	GLY	2.5
1	B	339	ALA	2.5
1	F	178	LEU	2.5
2	G	56	LEU	2.5
1	A	113	CYS	2.5
1	F	121	LEU	2.5
1	E	31	THR	2.5
1	F	164	ASP	2.5
1	A	247	PHE	2.5
1	E	296	TRP	2.5
2	G	55	LEU	2.5
1	F	276	GLY	2.4
1	F	169	LYS	2.4
1	F	190	ASP	2.4
2	H	48	GLU	2.4
1	A	313	ILE	2.4
2	C	37	LYS	2.4
1	A	159	TYR	2.4
2	G	83	LEU	2.4
2	D	102	PHE	2.4
1	B	310	LEU	2.4
2	H	49	PHE	2.4
1	E	21	ASP	2.4
1	A	176	ILE	2.4
1	F	171	LYS	2.4
1	B	33	GLU	2.3
1	E	217	PRO	2.3
1	F	201	LYS	2.3
2	D	65	LYS	2.3
1	B	383	TYR	2.3
1	E	123	LYS	2.3
1	F	214	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	280	VAL	2.3
1	F	143	VAL	2.3
1	F	191	ALA	2.3
2	D	67	ALA	2.3
1	F	85	ASP	2.3
1	A	94	CYS	2.3
1	A	105	LYS	2.3
1	A	119	VAL	2.3
2	H	35	SER	2.3
1	E	57	TYR	2.3
1	F	80	LYS	2.3
1	B	25	ASN	2.2
1	F	210	ALA	2.2
1	B	393	GLU	2.2
2	G	62	PHE	2.2
1	E	281	THR	2.2
1	F	251	PHE	2.2
1	B	366	THR	2.2
2	H	52	ALA	2.2
1	A	160	LYS	2.2
1	E	373	VAL	2.2
1	A	83	LEU	2.2
1	A	177	LEU	2.2
1	B	26	LEU	2.2
1	E	27	THR	2.2
1	F	228	ILE	2.2
1	E	357	GLY	2.2
1	A	333	PRO	2.2
1	A	58	TRP	2.2
1	E	348	PHE	2.1
1	E	52	LYS	2.1
1	E	346	GLY	2.1
1	B	369	ILE	2.1
1	B	386	ASN	2.1
2	H	47	ASN	2.1
1	F	78	PRO	2.1
1	E	330	PHE	2.1
2	H	91	LEU	2.1
1	A	103	GLU	2.1
1	E	344	ARG	2.1
1	A	161	GLU	2.1
1	B	35	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	59	ASP	2.1
1	E	45	ILE	2.1
1	B	354	LYS	2.1
1	F	281	THR	2.1
1	E	284	ALA	2.1
1	A	256	THR	2.0
1	F	108	VAL	2.0
1	A	165	ASN	2.0
2	H	44	ILE	2.0
1	B	260	GLU	2.0
1	E	191	ALA	2.0
1	F	162	VAL	2.0
1	B	362	ARG	2.0
1	F	270	LEU	2.0
1	B	361	ILE	2.0
1	E	327	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	LLP	E	234	24/25	0.93	0.26	79,128,147,154	0
1	LLP	F	234	24/25	0.95	0.21	63,92,100,105	0
1	LLP	B	234	24/25	0.96	0.21	59,80,91,95	0
1	LLP	A	234	24/25	0.98	0.22	29,65,85,92	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.