Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:54 pm BST

PDB ID	:	4ZAS
Title	:	Crystal structure of sugar aminotransferase CalS13 from Micromonospora echinospora
Authors	:	Wang, F.; Singh, S.; Miller, M.D.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on	:	2015-04-13
Resolution	:	2.47 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:

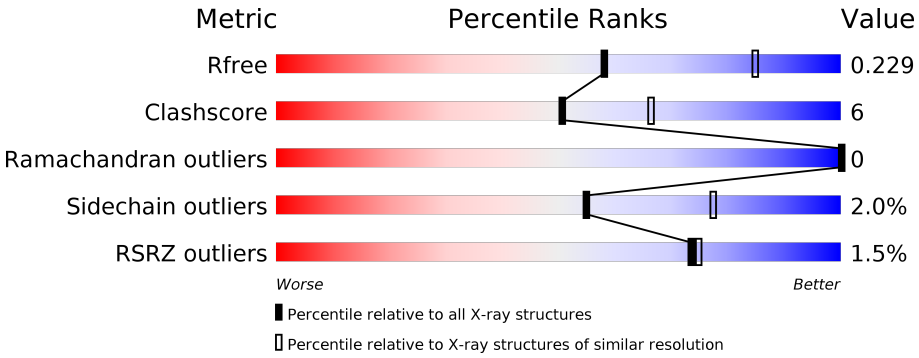
MolProbity	:	4.02b-467
Mogul	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 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 <=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	404	2% 79% 12% 9%
1	B	404	79% 12% • 9%
1	C	404	81% 10% • 9%
1	D	404	% 79% 12% 9%
1	E	404	% 77% 14% 9%
1	F	404	5% 78% 13% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17830 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 CalS13.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	P	S	0	0	0
			2868	1798	526	534	1	9			
1	B	369	Total	C	N	O	P	S	0	0	0
			2868	1798	526	534	1	9			
1	C	369	Total	C	N	O	P	S	0	0	0
			2868	1798	526	534	1	9			
1	D	369	Total	C	N	O	P	S	0	0	0
			2868	1798	526	534	1	9			
1	E	369	Total	C	N	O	P	S	0	0	0
			2868	1798	526	534	1	9			
1	F	369	Total	C	N	O	P	S	0	0	0
			2868	1798	526	534	1	9			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8KND8
A	-18	GLY	-	expression tag	UNP Q8KND8
A	-17	SER	-	expression tag	UNP Q8KND8
A	-16	SER	-	expression tag	UNP Q8KND8
A	-15	HIS	-	expression tag	UNP Q8KND8
A	-14	HIS	-	expression tag	UNP Q8KND8
A	-13	HIS	-	expression tag	UNP Q8KND8
A	-12	HIS	-	expression tag	UNP Q8KND8
A	-11	HIS	-	expression tag	UNP Q8KND8
A	-10	HIS	-	expression tag	UNP Q8KND8
A	-9	SER	-	expression tag	UNP Q8KND8
A	-8	SER	-	expression tag	UNP Q8KND8
A	-7	GLY	-	expression tag	UNP Q8KND8
A	-6	LEU	-	expression tag	UNP Q8KND8
A	-5	VAL	-	expression tag	UNP Q8KND8
A	-4	PRO	-	expression tag	UNP Q8KND8
A	-3	ARG	-	expression tag	UNP Q8KND8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8KND8
A	-1	SER	-	expression tag	UNP Q8KND8
A	0	HIS	-	expression tag	UNP Q8KND8
A	1	MET	-	expression tag	UNP Q8KND8
A	2	ALA	-	expression tag	UNP Q8KND8
A	3	THR	-	expression tag	UNP Q8KND8
A	4	SER	-	expression tag	UNP Q8KND8
A	5	GLU	-	expression tag	UNP Q8KND8
A	6	ARG	-	expression tag	UNP Q8KND8
A	7	GLY	-	expression tag	UNP Q8KND8
A	8	VAL	-	expression tag	UNP Q8KND8
B	-19	MET	-	expression tag	UNP Q8KND8
B	-18	GLY	-	expression tag	UNP Q8KND8
B	-17	SER	-	expression tag	UNP Q8KND8
B	-16	SER	-	expression tag	UNP Q8KND8
B	-15	HIS	-	expression tag	UNP Q8KND8
B	-14	HIS	-	expression tag	UNP Q8KND8
B	-13	HIS	-	expression tag	UNP Q8KND8
B	-12	HIS	-	expression tag	UNP Q8KND8
B	-11	HIS	-	expression tag	UNP Q8KND8
B	-10	HIS	-	expression tag	UNP Q8KND8
B	-9	SER	-	expression tag	UNP Q8KND8
B	-8	SER	-	expression tag	UNP Q8KND8
B	-7	GLY	-	expression tag	UNP Q8KND8
B	-6	LEU	-	expression tag	UNP Q8KND8
B	-5	VAL	-	expression tag	UNP Q8KND8
B	-4	PRO	-	expression tag	UNP Q8KND8
B	-3	ARG	-	expression tag	UNP Q8KND8
B	-2	GLY	-	expression tag	UNP Q8KND8
B	-1	SER	-	expression tag	UNP Q8KND8
B	0	HIS	-	expression tag	UNP Q8KND8
B	1	MET	-	expression tag	UNP Q8KND8
B	2	ALA	-	expression tag	UNP Q8KND8
B	3	THR	-	expression tag	UNP Q8KND8
B	4	SER	-	expression tag	UNP Q8KND8
B	5	GLU	-	expression tag	UNP Q8KND8
B	6	ARG	-	expression tag	UNP Q8KND8
B	7	GLY	-	expression tag	UNP Q8KND8
B	8	VAL	-	expression tag	UNP Q8KND8
C	-19	MET	-	expression tag	UNP Q8KND8
C	-18	GLY	-	expression tag	UNP Q8KND8
C	-17	SER	-	expression tag	UNP Q8KND8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP Q8KND8
C	-15	HIS	-	expression tag	UNP Q8KND8
C	-14	HIS	-	expression tag	UNP Q8KND8
C	-13	HIS	-	expression tag	UNP Q8KND8
C	-12	HIS	-	expression tag	UNP Q8KND8
C	-11	HIS	-	expression tag	UNP Q8KND8
C	-10	HIS	-	expression tag	UNP Q8KND8
C	-9	SER	-	expression tag	UNP Q8KND8
C	-8	SER	-	expression tag	UNP Q8KND8
C	-7	GLY	-	expression tag	UNP Q8KND8
C	-6	LEU	-	expression tag	UNP Q8KND8
C	-5	VAL	-	expression tag	UNP Q8KND8
C	-4	PRO	-	expression tag	UNP Q8KND8
C	-3	ARG	-	expression tag	UNP Q8KND8
C	-2	GLY	-	expression tag	UNP Q8KND8
C	-1	SER	-	expression tag	UNP Q8KND8
C	0	HIS	-	expression tag	UNP Q8KND8
C	1	MET	-	expression tag	UNP Q8KND8
C	2	ALA	-	expression tag	UNP Q8KND8
C	3	THR	-	expression tag	UNP Q8KND8
C	4	SER	-	expression tag	UNP Q8KND8
C	5	GLU	-	expression tag	UNP Q8KND8
C	6	ARG	-	expression tag	UNP Q8KND8
C	7	GLY	-	expression tag	UNP Q8KND8
C	8	VAL	-	expression tag	UNP Q8KND8
D	-19	MET	-	expression tag	UNP Q8KND8
D	-18	GLY	-	expression tag	UNP Q8KND8
D	-17	SER	-	expression tag	UNP Q8KND8
D	-16	SER	-	expression tag	UNP Q8KND8
D	-15	HIS	-	expression tag	UNP Q8KND8
D	-14	HIS	-	expression tag	UNP Q8KND8
D	-13	HIS	-	expression tag	UNP Q8KND8
D	-12	HIS	-	expression tag	UNP Q8KND8
D	-11	HIS	-	expression tag	UNP Q8KND8
D	-10	HIS	-	expression tag	UNP Q8KND8
D	-9	SER	-	expression tag	UNP Q8KND8
D	-8	SER	-	expression tag	UNP Q8KND8
D	-7	GLY	-	expression tag	UNP Q8KND8
D	-6	LEU	-	expression tag	UNP Q8KND8
D	-5	VAL	-	expression tag	UNP Q8KND8
D	-4	PRO	-	expression tag	UNP Q8KND8
D	-3	ARG	-	expression tag	UNP Q8KND8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q8KND8
D	-1	SER	-	expression tag	UNP Q8KND8
D	0	HIS	-	expression tag	UNP Q8KND8
D	1	MET	-	expression tag	UNP Q8KND8
D	2	ALA	-	expression tag	UNP Q8KND8
D	3	THR	-	expression tag	UNP Q8KND8
D	4	SER	-	expression tag	UNP Q8KND8
D	5	GLU	-	expression tag	UNP Q8KND8
D	6	ARG	-	expression tag	UNP Q8KND8
D	7	GLY	-	expression tag	UNP Q8KND8
D	8	VAL	-	expression tag	UNP Q8KND8
E	-19	MET	-	expression tag	UNP Q8KND8
E	-18	GLY	-	expression tag	UNP Q8KND8
E	-17	SER	-	expression tag	UNP Q8KND8
E	-16	SER	-	expression tag	UNP Q8KND8
E	-15	HIS	-	expression tag	UNP Q8KND8
E	-14	HIS	-	expression tag	UNP Q8KND8
E	-13	HIS	-	expression tag	UNP Q8KND8
E	-12	HIS	-	expression tag	UNP Q8KND8
E	-11	HIS	-	expression tag	UNP Q8KND8
E	-10	HIS	-	expression tag	UNP Q8KND8
E	-9	SER	-	expression tag	UNP Q8KND8
E	-8	SER	-	expression tag	UNP Q8KND8
E	-7	GLY	-	expression tag	UNP Q8KND8
E	-6	LEU	-	expression tag	UNP Q8KND8
E	-5	VAL	-	expression tag	UNP Q8KND8
E	-4	PRO	-	expression tag	UNP Q8KND8
E	-3	ARG	-	expression tag	UNP Q8KND8
E	-2	GLY	-	expression tag	UNP Q8KND8
E	-1	SER	-	expression tag	UNP Q8KND8
E	0	HIS	-	expression tag	UNP Q8KND8
E	1	MET	-	expression tag	UNP Q8KND8
E	2	ALA	-	expression tag	UNP Q8KND8
E	3	THR	-	expression tag	UNP Q8KND8
E	4	SER	-	expression tag	UNP Q8KND8
E	5	GLU	-	expression tag	UNP Q8KND8
E	6	ARG	-	expression tag	UNP Q8KND8
E	7	GLY	-	expression tag	UNP Q8KND8
E	8	VAL	-	expression tag	UNP Q8KND8
F	-19	MET	-	expression tag	UNP Q8KND8
F	-18	GLY	-	expression tag	UNP Q8KND8
F	-17	SER	-	expression tag	UNP Q8KND8

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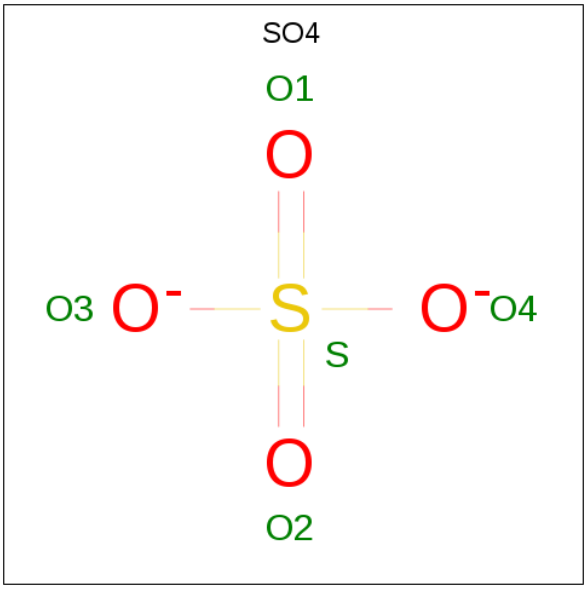
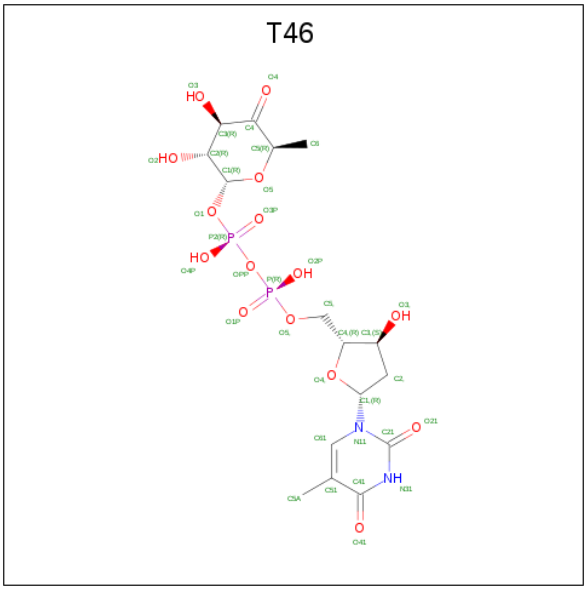
Chain	Residue	Modelled	Actual	Comment	Reference
F	-16	SER	-	expression tag	UNP Q8KND8
F	-15	HIS	-	expression tag	UNP Q8KND8
F	-14	HIS	-	expression tag	UNP Q8KND8
F	-13	HIS	-	expression tag	UNP Q8KND8
F	-12	HIS	-	expression tag	UNP Q8KND8
F	-11	HIS	-	expression tag	UNP Q8KND8
F	-10	HIS	-	expression tag	UNP Q8KND8
F	-9	SER	-	expression tag	UNP Q8KND8
F	-8	SER	-	expression tag	UNP Q8KND8
F	-7	GLY	-	expression tag	UNP Q8KND8
F	-6	LEU	-	expression tag	UNP Q8KND8
F	-5	VAL	-	expression tag	UNP Q8KND8
F	-4	PRO	-	expression tag	UNP Q8KND8
F	-3	ARG	-	expression tag	UNP Q8KND8
F	-2	GLY	-	expression tag	UNP Q8KND8
F	-1	SER	-	expression tag	UNP Q8KND8
F	0	HIS	-	expression tag	UNP Q8KND8
F	1	MET	-	expression tag	UNP Q8KND8
F	2	ALA	-	expression tag	UNP Q8KND8
F	3	THR	-	expression tag	UNP Q8KND8
F	4	SER	-	expression tag	UNP Q8KND8
F	5	GLU	-	expression tag	UNP Q8KND8
F	6	ARG	-	expression tag	UNP Q8KND8
F	7	GLY	-	expression tag	UNP Q8KND8
F	8	VAL	-	expression tag	UNP Q8KND8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



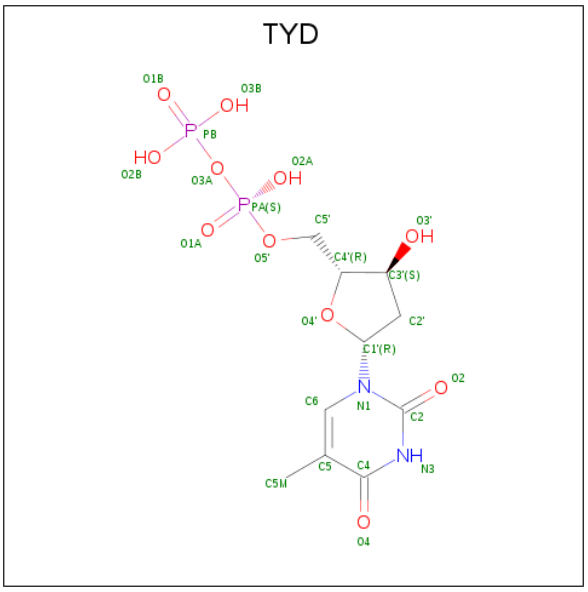
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is dTDP-4-keto-6-deoxyglucose (three-letter code: T46) (formula: $C_{16}H_{24}N_2O_{15}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 35 16 2 15 2	0	0

- Molecule 4 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	E	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	F	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 5 is water.

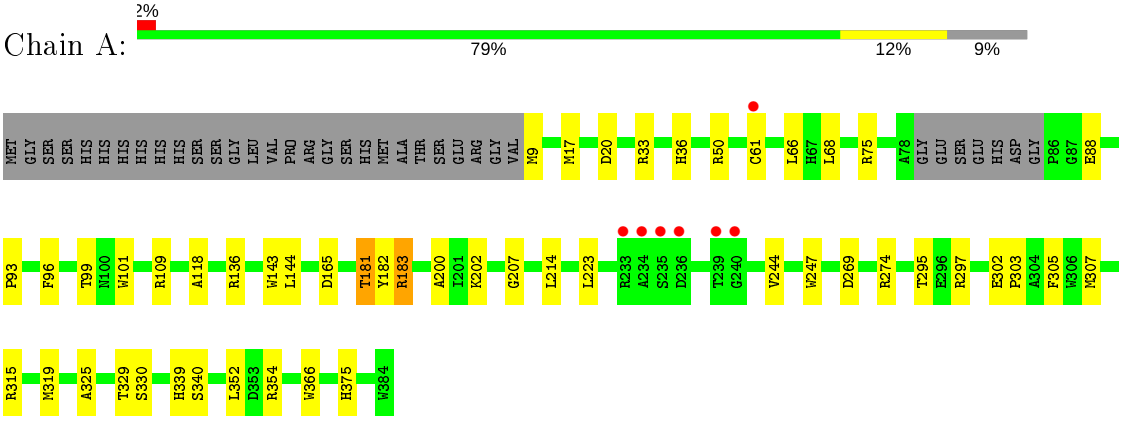
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	0
			95	95		
5	B	112	Total	O	0	0
			112	112		
5	C	69	Total	O	0	0
			69	69		
5	D	101	Total	O	0	0
			101	101		
5	E	67	Total	O	0	0
			67	67		
5	F	58	Total	O	0	0
			58	58		

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 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.

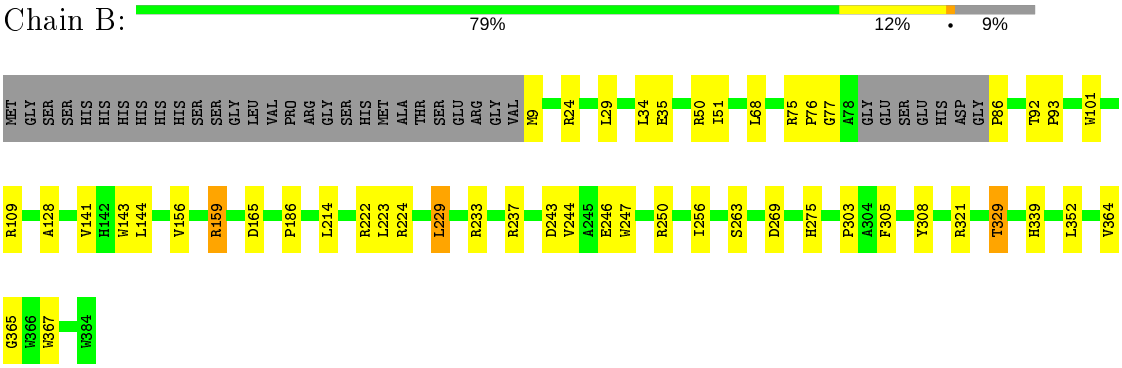
- Molecule 1: CalS13

Chain A:



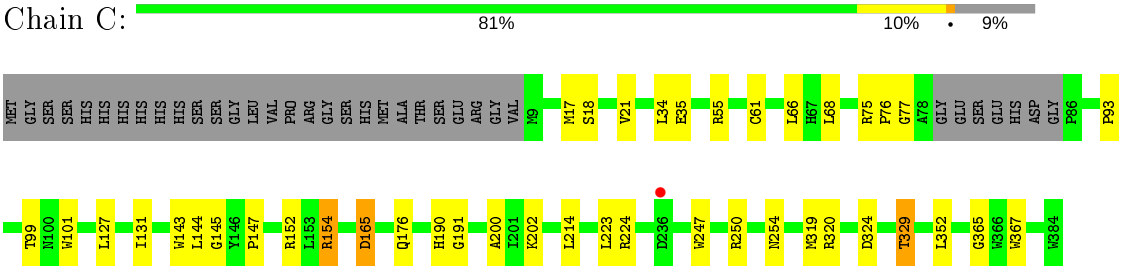
- Molecule 1: CalS13

Chain B:



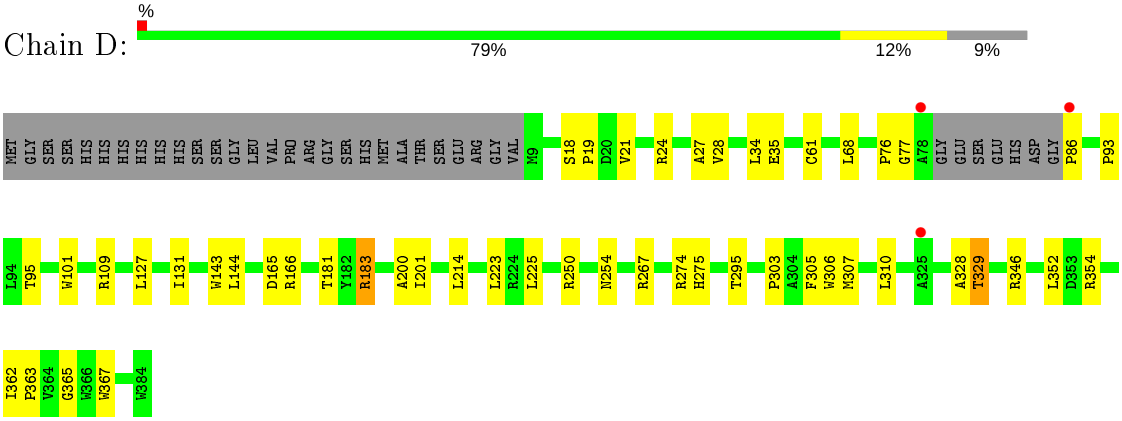
- Molecule 1: CalS13

Chain C:



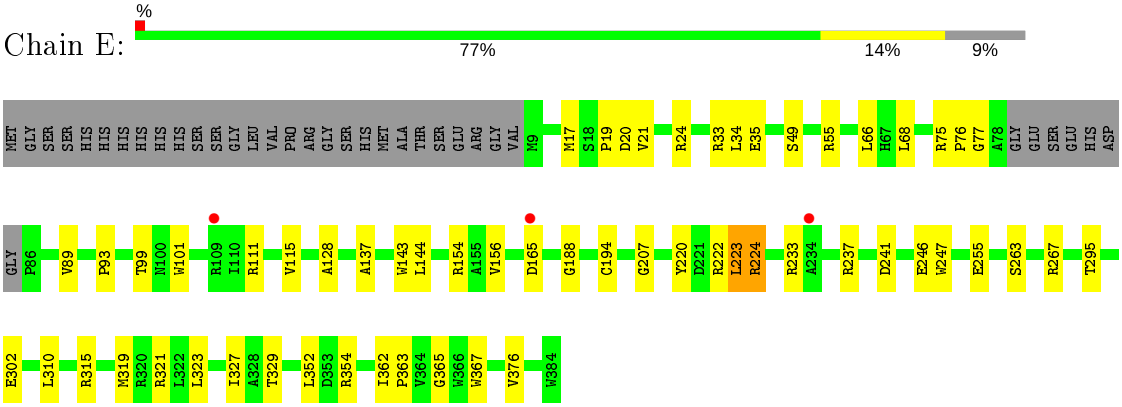
- Molecule 1: CalS13

Chain D:



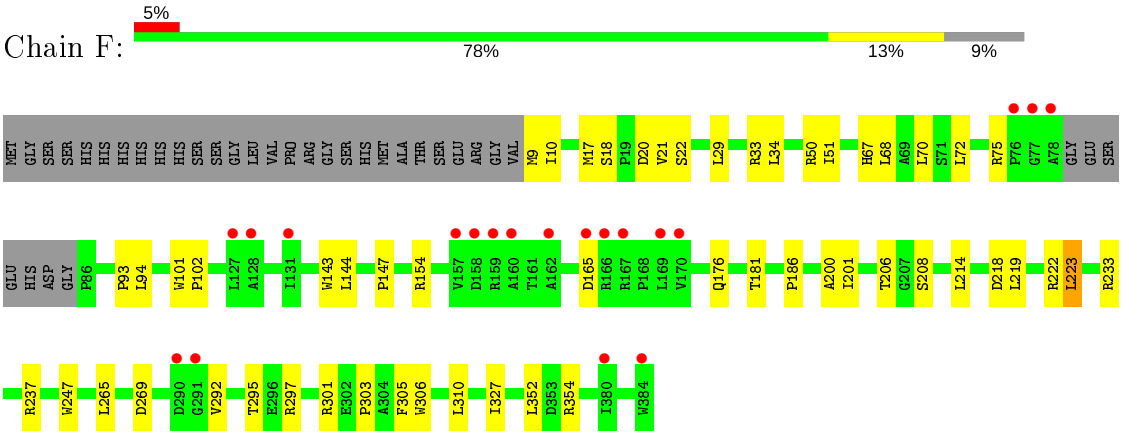
- Molecule 1: CalS13

Chain E:



- Molecule 1: CalS13

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.57Å 88.74Å 189.81Å 90.00° 96.22° 90.00°	Depositor
Resolution (Å)	43.19 – 2.47 44.37 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.19-2.47) 90.9 (44.37-2.47)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.173 , 0.229 0.173 , 0.229	Depositor DCC
R_{free} test set	2006 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å^2)	40.5	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17830	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: TYD, LLP, SO4, T46

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	0.44	0/2904	0.62	0/3956
1	B	0.44	0/2904	0.64	1/3956 (0.0%)
1	C	0.40	0/2904	0.59	0/3956
1	D	0.42	0/2904	0.61	0/3956
1	E	0.40	0/2904	0.60	0/3956
1	F	0.37	0/2904	0.57	0/3956
All	All	0.41	0/17424	0.60	1/23736 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	229	LEU	CA-CB-CG	-5.05	103.69	115.30

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	2868	0	2839	36	0
1	B	2868	0	2839	36	0
1	C	2868	0	2839	30	0
1	D	2868	0	2839	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2868	0	2839	40	0
1	F	2868	0	2839	36	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	B	35	0	22	2	0
4	D	25	0	13	0	0
4	E	25	0	13	2	0
4	F	25	0	13	0	0
5	A	95	0	0	8	0
5	B	112	0	0	11	0
5	C	69	0	0	4	0
5	D	101	0	0	8	0
5	E	67	0	0	9	0
5	F	58	0	0	7	0
All	All	17830	0	17095	197	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 (197) 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:319:MET:SD	5:E:653:HOH:O	2.34	0.84
1:B:9:MET:N	5:B:501:HOH:O	2.13	0.80
1:A:319:MET:SD	5:A:429:HOH:O	2.38	0.80
1:E:222:ARG:NH1	1:E:246:GLU:OE2	2.25	0.69
1:A:20:ASP:OD1	5:A:401:HOH:O	2.12	0.68
1:F:50:ARG:NH1	1:F:269:ASP:OD1	2.22	0.68
1:C:202:LLP:OP1	5:C:501:HOH:O	2.11	0.68
1:D:295:THR:HG21	5:D:697:HOH:O	1.95	0.67
1:E:302:GLU:HG3	5:E:666:HOH:O	1.94	0.67
1:E:75:ARG:NH2	1:E:247:TRP:O	2.28	0.66
1:C:93:PRO:HG2	1:C:352:LEU:HD22	1.79	0.65
1:B:222:ARG:NH1	1:B:246:GLU:OE2	2.29	0.64
1:F:94:LEU:HG	5:F:646:HOH:O	1.97	0.64
1:C:176:GLN:HE21	1:C:202:LLP:HO3	1.46	0.63
1:E:233:ARG:O	1:E:237:ARG:NH2	2.32	0.63
1:F:143:TRP:CD1	1:F:144:LEU:HG	2.34	0.63
1:D:329:THR:HB	5:D:653:HOH:O	1.99	0.62
1:E:68:LEU:HG	1:E:223:LEU:HG	1.81	0.62
1:A:75:ARG:NH2	1:A:247:TRP:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:TRP:CD1	1:E:144:LEU:HG	2.35	0.62
1:B:233:ARG:O	1:B:237:ARG:NH2	2.34	0.61
1:B:86:PRO:O	5:B:502:HOH:O	2.16	0.61
1:C:152:ARG:NH2	5:C:503:HOH:O	2.34	0.61
1:C:329:THR:HB	5:C:516:HOH:O	2.00	0.61
1:B:75:ARG:NH2	1:B:247:TRP:O	2.33	0.60
1:F:201:ILE:HG13	1:F:306:TRP:HZ2	1.67	0.60
1:A:295:THR:HG21	5:A:491:HOH:O	2.01	0.60
1:D:310:LEU:HD12	1:D:362:ILE:HD12	1.84	0.60
1:E:295:THR:HG21	5:E:667:HOH:O	2.01	0.59
1:E:241:ASP:OD1	5:E:602:HOH:O	2.16	0.59
1:A:136:ARG:NH1	5:A:402:HOH:O	2.22	0.59
1:B:128:ALA:HB2	1:B:156:VAL:HG13	1.85	0.59
1:B:329:THR:HB	5:B:552:HOH:O	2.03	0.59
1:F:218:ASP:HB3	5:F:631:HOH:O	2.02	0.59
1:D:28:VAL:HG23	5:D:601:HOH:O	2.01	0.59
1:F:295:THR:HB	1:F:297:ARG:HH12	1.68	0.58
1:E:89:VAL:HG22	1:E:137:ALA:HB3	1.85	0.58
1:C:214:LEU:HD11	1:C:223:LEU:HD22	1.86	0.58
1:A:9:MET:N	5:A:405:HOH:O	2.36	0.58
1:B:51:ILE:O	1:B:186:PRO:HG2	2.03	0.58
1:A:68:LEU:HG	1:A:223:LEU:HG	1.86	0.58
1:B:143:TRP:CD1	1:B:144:LEU:HG	2.40	0.57
1:F:93:PRO:HG2	1:F:352:LEU:HD22	1.87	0.57
1:A:33:ARG:HH12	1:A:36:HIS:HB2	1.69	0.57
1:E:111:ARG:HD3	5:E:665:HOH:O	2.02	0.57
1:F:222:ARG:NE	5:F:604:HOH:O	2.30	0.56
1:B:214:LEU:HD11	1:B:223:LEU:HD22	1.86	0.56
1:D:68:LEU:HG	1:D:223:LEU:HG	1.86	0.56
1:B:68:LEU:HG	1:B:223:LEU:HG	1.88	0.56
1:C:18:SER:HB3	1:C:21:VAL:HG23	1.87	0.56
1:C:68:LEU:HG	1:C:223:LEU:HG	1.86	0.56
1:D:214:LEU:HD11	1:D:223:LEU:HD22	1.88	0.56
1:E:21:VAL:HG12	1:F:29:LEU:HD13	1.87	0.56
1:D:18:SER:HB3	1:D:21:VAL:HG23	1.87	0.55
5:B:505:HOH:O	1:D:86:PRO:HB2	2.06	0.55
1:B:93:PRO:HG2	1:B:352:LEU:HD22	1.89	0.55
1:E:93:PRO:HG2	1:E:352:LEU:HD22	1.87	0.55
1:F:75:ARG:NH2	1:F:247:TRP:O	2.39	0.54
1:C:365:GLY:HA3	1:C:367:TRP:CZ3	2.42	0.54
1:A:214:LEU:HD11	1:A:223:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:ARG:NH2	5:E:601:HOH:O	2.06	0.53
1:A:66:LEU:HD13	1:A:99:THR:HA	1.91	0.53
1:B:24:ARG:HD2	1:B:263:SER:OG	2.09	0.53
1:E:128:ALA:HB2	1:E:156:VAL:HG13	1.91	0.53
1:A:200:ALA:HB2	1:B:35:GLU:HG3	1.90	0.52
1:D:34:LEU:O	1:D:254:ASN:HB2	2.09	0.52
1:A:93:PRO:HG2	1:A:352:LEU:HD22	1.91	0.52
1:D:143:TRP:CD1	1:D:144:LEU:HG	2.45	0.52
1:B:250:ARG:NH1	5:B:504:HOH:O	2.33	0.52
1:B:76:PRO:HD2	5:B:604:HOH:O	2.11	0.51
1:F:72:LEU:HD13	1:F:219:LEU:HD22	1.92	0.51
1:A:143:TRP:CD1	1:A:144:LEU:HG	2.45	0.51
1:F:20:ASP:OD2	5:F:601:HOH:O	2.18	0.51
3:B:402:T46:O5,	3:B:402:T46:H9	2.10	0.51
1:B:76:PRO:N	1:B:77:GLY:HA3	2.24	0.51
1:E:354:ARG:NH2	5:E:603:HOH:O	2.22	0.51
1:D:354:ARG:HD3	5:D:694:HOH:O	2.09	0.51
1:C:200:ALA:HB2	1:D:35:GLU:HG3	1.92	0.51
1:F:22:SER:N	5:F:611:HOH:O	2.43	0.51
1:F:50:ARG:NH2	1:F:265:LEU:O	2.44	0.51
1:E:365:GLY:HA3	1:E:367:TRP:CH2	2.46	0.50
1:C:165:ASP:N	5:C:505:HOH:O	2.44	0.50
1:B:29:LEU:HD21	1:B:256:ILE:HD11	1.93	0.50
1:C:143:TRP:CD1	1:C:144:LEU:HG	2.46	0.50
1:E:188:GLY:HA2	1:E:194:CYS:SG	2.52	0.50
1:F:354:ARG:HG2	1:F:354:ARG:O	2.12	0.50
1:C:154:ARG:HH22	1:C:191:GLY:HA3	1.77	0.49
1:C:154:ARG:NH1	1:C:190:HIS:O	2.45	0.49
1:F:10:ILE:HD12	1:F:327:ILE:HG12	1.94	0.49
1:F:147:PRO:HB2	1:F:301:ARG:HD3	1.94	0.49
1:E:66:LEU:HD13	1:E:99:THR:HA	1.93	0.49
1:B:109:ARG:HD3	5:B:609:HOH:O	2.13	0.49
1:D:144:LEU:HD22	1:D:307:MET:HB2	1.95	0.48
1:D:365:GLY:HA3	1:D:367:TRP:CZ3	2.47	0.48
1:B:50:ARG:NH1	1:B:269:ASP:OD1	2.46	0.48
1:D:76:PRO:N	1:D:77:GLY:HA3	2.29	0.48
1:E:33:ARG:NH2	4:E:500:TYD:H2'2	2.28	0.48
1:D:27:ALA:HB3	5:D:601:HOH:O	2.13	0.48
1:E:365:GLY:HA3	1:E:367:TRP:CZ3	2.49	0.48
1:D:201:ILE:HG13	1:D:306:TRP:HZ2	1.78	0.48
1:B:303:PRO:HB2	1:B:305:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ARG:NH1	5:D:605:HOH:O	2.46	0.48
1:D:93:PRO:HG2	1:D:352:LEU:HD22	1.95	0.48
1:F:214:LEU:HD11	1:F:223:LEU:HD22	1.95	0.48
1:A:274:ARG:NH2	5:A:406:HOH:O	2.37	0.48
1:F:67:HIS:HA	1:F:102:PRO:HB3	1.95	0.48
1:B:92:THR:HG22	5:B:503:HOH:O	2.13	0.47
1:C:61:CYS:SG	1:D:250:ARG:HG3	2.54	0.47
1:D:346:ARG:HD3	5:D:698:HOH:O	2.14	0.47
1:B:275:HIS:CE1	1:B:365:GLY:HA2	2.49	0.47
1:E:327:ILE:HD13	1:E:376:VAL:HA	1.97	0.47
1:C:75:ARG:NH2	1:C:247:TRP:O	2.46	0.47
1:F:51:ILE:O	1:F:186:PRO:HG2	2.15	0.47
1:D:275:HIS:CE1	1:D:365:GLY:HA2	2.50	0.47
1:D:19:PRO:HD2	1:D:267:ARG:HE	1.80	0.47
1:A:17:MET:CE	1:B:34:LEU:HD11	2.46	0.46
1:A:61:CYS:SG	1:B:250:ARG:HG3	2.56	0.46
1:C:127:LEU:O	1:C:131:ILE:HG13	2.15	0.46
1:A:182:TYR:CE2	1:A:183:ARG:HG3	2.50	0.46
1:C:176:GLN:NE2	1:C:202:LLP:O3	2.39	0.46
1:C:76:PRO:N	1:C:77:GLY:HA3	2.30	0.46
1:C:320:ARG:NH1	1:C:324:ASP:OD1	2.49	0.46
1:B:75:ARG:HD3	5:B:590:HOH:O	2.16	0.46
1:E:35:GLU:HG3	1:F:200:ALA:HB2	1.97	0.46
1:F:10:ILE:HA	5:F:602:HOH:O	2.15	0.45
1:F:233:ARG:HA	1:F:237:ARG:HH21	1.81	0.45
1:F:292:VAL:HG13	1:F:310:LEU:HD22	1.98	0.45
1:D:303:PRO:HB2	1:D:305:PHE:CE2	2.51	0.45
1:E:49:SER:HB3	5:E:641:HOH:O	2.16	0.45
1:E:207:GLY:HA2	1:F:34:LEU:HD13	1.97	0.45
1:A:207:GLY:HA2	1:B:34:LEU:HD13	1.97	0.45
1:D:274:ARG:NH2	5:D:604:HOH:O	2.41	0.45
1:E:24:ARG:HD2	1:E:263:SER:OG	2.17	0.44
1:B:365:GLY:HA3	1:B:367:TRP:CZ3	2.52	0.44
1:D:183:ARG:NH2	5:E:601:HOH:O	2.50	0.44
1:C:34:LEU:O	1:C:254:ASN:HB2	2.18	0.44
1:A:50:ARG:NH1	1:A:269:ASP:OD1	2.43	0.44
1:A:274:ARG:NH1	1:A:366:TRP:O	2.50	0.44
1:B:141:VAL:HG23	5:B:503:HOH:O	2.17	0.44
1:D:183:ARG:HH11	1:E:20:ASP:CG	2.21	0.44
1:E:223:LEU:HD12	1:E:223:LEU:HA	1.64	0.44
1:E:33:ARG:O	1:E:255:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:O	1:A:319:MET:HG3	2.17	0.44
1:A:340:SER:OG	1:B:243:ASP:OD2	2.29	0.44
1:E:19:PRO:HD2	1:E:267:ARG:HE	1.82	0.44
1:A:181:THR:HG22	1:A:302:GLU:HB2	1.99	0.43
1:B:159:ARG:NH2	5:B:508:HOH:O	2.47	0.43
1:B:365:GLY:HA3	1:B:367:TRP:CH2	2.53	0.43
1:C:66:LEU:HD13	1:C:99:THR:HA	2.01	0.43
1:F:206:THR:OG1	1:F:208:SER:O	2.23	0.43
1:B:308:TYR:HB2	1:B:364:VAL:HB	2.00	0.43
1:D:127:LEU:O	1:D:131:ILE:HG13	2.19	0.43
1:C:365:GLY:HA3	1:C:367:TRP:CH2	2.54	0.43
1:F:68:LEU:HG	1:F:223:LEU:HG	2.00	0.43
1:A:244:VAL:HG23	1:B:339:HIS:CE1	2.54	0.43
1:C:145:GLY:O	1:C:147:PRO:HD3	2.18	0.43
1:D:95:THR:HA	1:D:143:TRP:CZ3	2.54	0.43
1:E:17:MET:CE	1:F:34:LEU:HD11	2.49	0.43
1:E:315:ARG:O	1:E:319:MET:HG3	2.18	0.43
4:E:500:TYD:O5'	4:E:500:TYD:H6	2.19	0.42
1:F:144:LEU:N	1:F:176:GLN:OE1	2.45	0.42
1:E:76:PRO:N	1:E:77:GLY:HA3	2.33	0.42
1:D:223:LEU:HD12	1:D:223:LEU:HA	1.85	0.42
1:F:303:PRO:HB2	1:F:305:PHE:CE2	2.55	0.42
1:C:319:MET:HG2	1:C:329:THR:HG21	2.01	0.42
1:A:136:ARG:HD3	5:A:402:HOH:O	2.19	0.42
1:F:9:MET:O	5:F:602:HOH:O	2.22	0.42
1:A:144:LEU:HD22	1:A:307:MET:HB2	2.02	0.42
1:F:18:SER:O	1:F:21:VAL:HG23	2.19	0.42
1:E:34:LEU:HD11	1:F:17:MET:CE	2.50	0.42
1:A:330:SER:HA	5:A:429:HOH:O	2.20	0.41
1:D:365:GLY:HA3	1:D:367:TRP:CH2	2.55	0.41
1:C:55:ARG:HD2	1:C:55:ARG:HH11	1.65	0.41
1:D:328:ALA:O	1:D:363:PRO:HD3	2.20	0.41
1:E:220:TYR:O	1:E:224:ARG:HB2	2.21	0.41
1:F:147:PRO:HG2	1:F:301:ARG:HB2	2.02	0.41
1:A:118:ALA:O	1:A:295:THR:HG23	2.20	0.41
1:A:339:HIS:CE1	1:B:244:VAL:HG23	2.55	0.41
1:A:354:ARG:HA	1:A:354:ARG:HD2	1.75	0.41
1:E:323:LEU:HA	1:E:323:LEU:HD12	1.84	0.41
1:E:310:LEU:HD12	1:E:362:ILE:HD12	2.03	0.41
1:A:96:PHE:CZ	1:B:229:LEU:HD13	2.56	0.41
1:C:17:MET:SD	1:C:21:VAL:HG21	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ARG:HH11	1:E:55:ARG:HD2	1.72	0.41
1:F:201:ILE:HG13	1:F:306:TRP:CZ2	2.52	0.41
1:C:35:GLU:HG3	1:D:200:ALA:HB2	2.02	0.41
1:C:250:ARG:HG3	1:D:61:CYS:SG	2.61	0.41
1:F:70:LEU:HD12	1:F:102:PRO:HB2	2.03	0.41
1:A:202:LLP:H4'1	3:B:402:T46:O4	2.21	0.41
1:A:303:PRO:HB2	1:A:305:PHE:CE2	2.56	0.40
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.80	0.40
1:A:295:THR:HB	1:A:297:ARG:HH12	1.86	0.40
1:D:225:LEU:HA	1:D:225:LEU:HD23	1.85	0.40
1:A:88:GLU:HG2	1:A:109:ARG:HB2	2.03	0.40
1:A:325:ALA:HB1	1:A:375:HIS:HE2	1.86	0.40
1:E:115:VAL:HG21	1:E:352:LEU:HD13	2.03	0.40
1:E:362:ILE:HA	1:E:363:PRO:HD3	1.98	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	364/404 (90%)	355 (98%)	9 (2%)	0	100	100
1	B	364/404 (90%)	354 (97%)	10 (3%)	0	100	100
1	C	364/404 (90%)	355 (98%)	9 (2%)	0	100	100
1	D	364/404 (90%)	355 (98%)	9 (2%)	0	100	100
1	E	364/404 (90%)	355 (98%)	9 (2%)	0	100	100
1	F	364/404 (90%)	356 (98%)	8 (2%)	0	100	100
All	All	2184/2424 (90%)	2130 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	297/325 (91%)	292 (98%)	5 (2%)	60	81
1	B	297/325 (91%)	291 (98%)	6 (2%)	55	77
1	C	297/325 (91%)	292 (98%)	5 (2%)	60	81
1	D	297/325 (91%)	290 (98%)	7 (2%)	49	72
1	E	297/325 (91%)	290 (98%)	7 (2%)	49	72
1	F	297/325 (91%)	291 (98%)	6 (2%)	55	77
All	All	1782/1950 (91%)	1746 (98%)	36 (2%)	55	77

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	TRP
1	A	165	ASP
1	A	181	THR
1	A	183	ARG
1	A	329	THR
1	B	101	TRP
1	B	159	ARG
1	B	165	ASP
1	B	224	ARG
1	B	321	ARG
1	B	329	THR
1	C	101	TRP
1	C	154	ARG
1	C	165	ASP
1	C	224	ARG
1	C	329	THR
1	D	24	ARG
1	D	101	TRP
1	D	109	ARG
1	D	165	ASP
1	D	181	THR
1	D	183	ARG

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Mol	Chain	Res	Type
1	D	329	THR
1	E	101	TRP
1	E	154	ARG
1	E	165	ASP
1	E	223	LEU
1	E	224	ARG
1	E	321	ARG
1	E	329	THR
1	F	33	ARG
1	F	101	TRP
1	F	154	ARG
1	F	165	ASP
1	F	181	THR
1	F	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

Mogul failed to run properly - this section is therefore empty.

5.5 Carbohydrates

Mogul failed to run properly - this section is therefore empty.

5.6 Ligand geometry

Mogul failed to run properly - this section is therefore empty.

5.7 Other polymers

Mogul failed to run properly - this section is therefore empty.

5.8 Polymer linkage issues

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	368/404 (91%)	-0.25	7 (1%) 66 68	32, 47, 76, 140	0
1	B	368/404 (91%)	-0.40	0 100 100	29, 47, 69, 88	0
1	C	368/404 (91%)	-0.10	1 (0%) 94 94	38, 57, 88, 119	0
1	D	368/404 (91%)	-0.31	3 (0%) 86 87	35, 50, 79, 111	0
1	E	368/404 (91%)	-0.21	3 (0%) 86 87	38, 59, 87, 125	0
1	F	368/404 (91%)	0.24	20 (5%) 25 26	40, 73, 107, 127	0
All	All	2208/2424 (91%)	-0.17	34 (1%) 73 75	29, 54, 92, 140	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	SER	4.6
1	A	236	ASP	4.4
1	F	127	LEU	3.8
1	F	128	ALA	3.7
1	F	77	GLY	3.6
1	F	162	ALA	3.6
1	F	380	ILE	3.6
1	A	239	THR	3.2
1	F	157	VAL	3.2
1	F	384	TRP	3.1
1	F	159	ARG	3.1
1	A	240	GLY	3.1
1	F	165	ASP	2.9
1	F	291	GLY	2.9
1	A	233	ARG	2.9
1	D	78	ALA	2.9
1	E	234	ALA	2.8
1	C	236	ASP	2.8
1	E	109	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	167	ARG	2.7
1	F	169	LEU	2.7
1	F	166	ARG	2.7
1	F	78	ALA	2.5
1	A	234	ALA	2.4
1	D	325	ALA	2.4
1	F	290	ASP	2.3
1	F	170	VAL	2.3
1	F	160	ALA	2.3
1	F	131	ILE	2.3
1	F	76	PRO	2.2
1	A	61	CYS	2.2
1	E	165	ASP	2.2
1	D	86	PRO	2.0
1	F	158	ASP	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	202	24/25	0.97	0.21	40,53,61,64	0
1	LLP	C	202	24/25	0.97	0.15	37,51,63,66	0
1	LLP	A	202	24/25	0.97	0.19	31,44,49,54	0
1	LLP	F	202	24/25	0.97	0.20	51,65,78,80	0
1	LLP	B	202	24/25	0.97	0.17	27,47,65,72	0
1	LLP	D	202	24/25	0.97	0.17	41,50,62,69	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	TYD	F	500	25/25	0.85	0.21	47,92,103,105	25
4	TYD	E	500	25/25	0.87	0.20	58,85,101,107	25
3	T46	B	402	35/35	0.88	0.22	50,64,88,95	35
4	TYD	D	500	25/25	0.91	0.17	52,70,101,108	0
2	SO4	C	401	5/5	0.93	0.35	127,130,131,133	0
2	SO4	B	401	5/5	0.97	0.13	73,76,80,90	0

6.5 Other polymers (i)

There are no such residues in this entry.