wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 01:26 AM EST

PDB ID	:	8EQW
Title	:	Crystal structure of Fub7
Authors	:	Hai, Y.
Deposited on	:	2022-10-10
Resolution	:	1.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

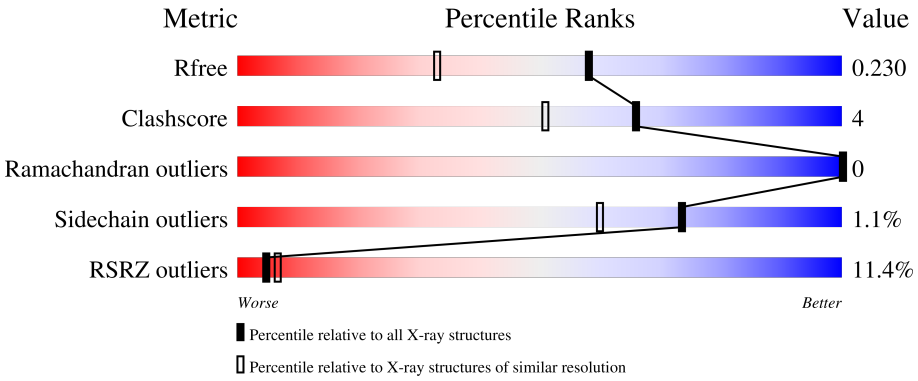
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	450	10% 84% 10% 6%
1	B	450	8% 81% 9% • 10%
1	C	450	11% 84% 9% 7%
1	D	450	12% 84% 8% 8%
1	E	450	11% 85% 9% 6%

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Mol	Chain	Length	Quality of chain
1	F	450	12% 86% 8% 6%
1	G	450	11% 79% 12% • 8%
1	H	450	9% 82% 12% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 27419 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 Sulfhydrylase FUB7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	P	S	0	0	0
			3259	2070	561	620	1	7			
1	B	407	Total	C	N	O	P	S	0	0	0
			3143	2000	538	597	1	7			
1	C	418	Total	C	N	O	P	S	0	0	0
			3220	2046	554	612	1	7			
1	D	414	Total	C	N	O	P	S	0	0	0
			3198	2035	548	607	1	7			
1	E	424	Total	C	N	O	P	S	0	0	0
			3271	2075	563	625	1	7			
1	F	424	Total	C	N	O	P	S	0	0	0
			3272	2074	563	627	1	7			
1	G	415	Total	C	N	O	P	S	0	1	0
			3210	2042	552	608	1	7			
1	H	426	Total	C	N	O	P	S	0	0	0
			3289	2085	566	630	1	7			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP S0DUX5
A	-15	GLY	-	expression tag	UNP S0DUX5
A	-14	SER	-	expression tag	UNP S0DUX5
A	-13	SER	-	expression tag	UNP S0DUX5
A	-12	HIS	-	expression tag	UNP S0DUX5
A	-11	HIS	-	expression tag	UNP S0DUX5
A	-10	HIS	-	expression tag	UNP S0DUX5
A	-9	HIS	-	expression tag	UNP S0DUX5
A	-8	HIS	-	expression tag	UNP S0DUX5
A	-7	HIS	-	expression tag	UNP S0DUX5
A	-6	GLU	-	expression tag	UNP S0DUX5
A	-5	ASN	-	expression tag	UNP S0DUX5
A	-4	LEU	-	expression tag	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP S0DUX5
A	-2	PHE	-	expression tag	UNP S0DUX5
A	-1	GLN	-	expression tag	UNP S0DUX5
A	0	SER	-	expression tag	UNP S0DUX5
A	1	ASN	-	expression tag	UNP S0DUX5
B	-16	MET	-	initiating methionine	UNP S0DUX5
B	-15	GLY	-	expression tag	UNP S0DUX5
B	-14	SER	-	expression tag	UNP S0DUX5
B	-13	SER	-	expression tag	UNP S0DUX5
B	-12	HIS	-	expression tag	UNP S0DUX5
B	-11	HIS	-	expression tag	UNP S0DUX5
B	-10	HIS	-	expression tag	UNP S0DUX5
B	-9	HIS	-	expression tag	UNP S0DUX5
B	-8	HIS	-	expression tag	UNP S0DUX5
B	-7	HIS	-	expression tag	UNP S0DUX5
B	-6	GLU	-	expression tag	UNP S0DUX5
B	-5	ASN	-	expression tag	UNP S0DUX5
B	-4	LEU	-	expression tag	UNP S0DUX5
B	-3	TYR	-	expression tag	UNP S0DUX5
B	-2	PHE	-	expression tag	UNP S0DUX5
B	-1	GLN	-	expression tag	UNP S0DUX5
B	0	SER	-	expression tag	UNP S0DUX5
B	1	ASN	-	expression tag	UNP S0DUX5
C	-16	MET	-	initiating methionine	UNP S0DUX5
C	-15	GLY	-	expression tag	UNP S0DUX5
C	-14	SER	-	expression tag	UNP S0DUX5
C	-13	SER	-	expression tag	UNP S0DUX5
C	-12	HIS	-	expression tag	UNP S0DUX5
C	-11	HIS	-	expression tag	UNP S0DUX5
C	-10	HIS	-	expression tag	UNP S0DUX5
C	-9	HIS	-	expression tag	UNP S0DUX5
C	-8	HIS	-	expression tag	UNP S0DUX5
C	-7	HIS	-	expression tag	UNP S0DUX5
C	-6	GLU	-	expression tag	UNP S0DUX5
C	-5	ASN	-	expression tag	UNP S0DUX5
C	-4	LEU	-	expression tag	UNP S0DUX5
C	-3	TYR	-	expression tag	UNP S0DUX5
C	-2	PHE	-	expression tag	UNP S0DUX5
C	-1	GLN	-	expression tag	UNP S0DUX5
C	0	SER	-	expression tag	UNP S0DUX5
C	1	ASN	-	expression tag	UNP S0DUX5
D	-16	MET	-	initiating methionine	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	expression tag	UNP S0DUX5
D	-14	SER	-	expression tag	UNP S0DUX5
D	-13	SER	-	expression tag	UNP S0DUX5
D	-12	HIS	-	expression tag	UNP S0DUX5
D	-11	HIS	-	expression tag	UNP S0DUX5
D	-10	HIS	-	expression tag	UNP S0DUX5
D	-9	HIS	-	expression tag	UNP S0DUX5
D	-8	HIS	-	expression tag	UNP S0DUX5
D	-7	HIS	-	expression tag	UNP S0DUX5
D	-6	GLU	-	expression tag	UNP S0DUX5
D	-5	ASN	-	expression tag	UNP S0DUX5
D	-4	LEU	-	expression tag	UNP S0DUX5
D	-3	TYR	-	expression tag	UNP S0DUX5
D	-2	PHE	-	expression tag	UNP S0DUX5
D	-1	GLN	-	expression tag	UNP S0DUX5
D	0	SER	-	expression tag	UNP S0DUX5
D	1	ASN	-	expression tag	UNP S0DUX5
E	-16	MET	-	initiating methionine	UNP S0DUX5
E	-15	GLY	-	expression tag	UNP S0DUX5
E	-14	SER	-	expression tag	UNP S0DUX5
E	-13	SER	-	expression tag	UNP S0DUX5
E	-12	HIS	-	expression tag	UNP S0DUX5
E	-11	HIS	-	expression tag	UNP S0DUX5
E	-10	HIS	-	expression tag	UNP S0DUX5
E	-9	HIS	-	expression tag	UNP S0DUX5
E	-8	HIS	-	expression tag	UNP S0DUX5
E	-7	HIS	-	expression tag	UNP S0DUX5
E	-6	GLU	-	expression tag	UNP S0DUX5
E	-5	ASN	-	expression tag	UNP S0DUX5
E	-4	LEU	-	expression tag	UNP S0DUX5
E	-3	TYR	-	expression tag	UNP S0DUX5
E	-2	PHE	-	expression tag	UNP S0DUX5
E	-1	GLN	-	expression tag	UNP S0DUX5
E	0	SER	-	expression tag	UNP S0DUX5
E	1	ASN	-	expression tag	UNP S0DUX5
F	-16	MET	-	initiating methionine	UNP S0DUX5
F	-15	GLY	-	expression tag	UNP S0DUX5
F	-14	SER	-	expression tag	UNP S0DUX5
F	-13	SER	-	expression tag	UNP S0DUX5
F	-12	HIS	-	expression tag	UNP S0DUX5
F	-11	HIS	-	expression tag	UNP S0DUX5
F	-10	HIS	-	expression tag	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP S0DUX5
F	-8	HIS	-	expression tag	UNP S0DUX5
F	-7	HIS	-	expression tag	UNP S0DUX5
F	-6	GLU	-	expression tag	UNP S0DUX5
F	-5	ASN	-	expression tag	UNP S0DUX5
F	-4	LEU	-	expression tag	UNP S0DUX5
F	-3	TYR	-	expression tag	UNP S0DUX5
F	-2	PHE	-	expression tag	UNP S0DUX5
F	-1	GLN	-	expression tag	UNP S0DUX5
F	0	SER	-	expression tag	UNP S0DUX5
F	1	ASN	-	expression tag	UNP S0DUX5
G	-16	MET	-	initiating methionine	UNP S0DUX5
G	-15	GLY	-	expression tag	UNP S0DUX5
G	-14	SER	-	expression tag	UNP S0DUX5
G	-13	SER	-	expression tag	UNP S0DUX5
G	-12	HIS	-	expression tag	UNP S0DUX5
G	-11	HIS	-	expression tag	UNP S0DUX5
G	-10	HIS	-	expression tag	UNP S0DUX5
G	-9	HIS	-	expression tag	UNP S0DUX5
G	-8	HIS	-	expression tag	UNP S0DUX5
G	-7	HIS	-	expression tag	UNP S0DUX5
G	-6	GLU	-	expression tag	UNP S0DUX5
G	-5	ASN	-	expression tag	UNP S0DUX5
G	-4	LEU	-	expression tag	UNP S0DUX5
G	-3	TYR	-	expression tag	UNP S0DUX5
G	-2	PHE	-	expression tag	UNP S0DUX5
G	-1	GLN	-	expression tag	UNP S0DUX5
G	0	SER	-	expression tag	UNP S0DUX5
G	1	ASN	-	expression tag	UNP S0DUX5
H	-16	MET	-	initiating methionine	UNP S0DUX5
H	-15	GLY	-	expression tag	UNP S0DUX5
H	-14	SER	-	expression tag	UNP S0DUX5
H	-13	SER	-	expression tag	UNP S0DUX5
H	-12	HIS	-	expression tag	UNP S0DUX5
H	-11	HIS	-	expression tag	UNP S0DUX5
H	-10	HIS	-	expression tag	UNP S0DUX5
H	-9	HIS	-	expression tag	UNP S0DUX5
H	-8	HIS	-	expression tag	UNP S0DUX5
H	-7	HIS	-	expression tag	UNP S0DUX5
H	-6	GLU	-	expression tag	UNP S0DUX5
H	-5	ASN	-	expression tag	UNP S0DUX5
H	-4	LEU	-	expression tag	UNP S0DUX5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	TYR	-	expression tag	UNP S0DUX5
H	-2	PHE	-	expression tag	UNP S0DUX5
H	-1	GLN	-	expression tag	UNP S0DUX5
H	0	SER	-	expression tag	UNP S0DUX5
H	1	ASN	-	expression tag	UNP S0DUX5

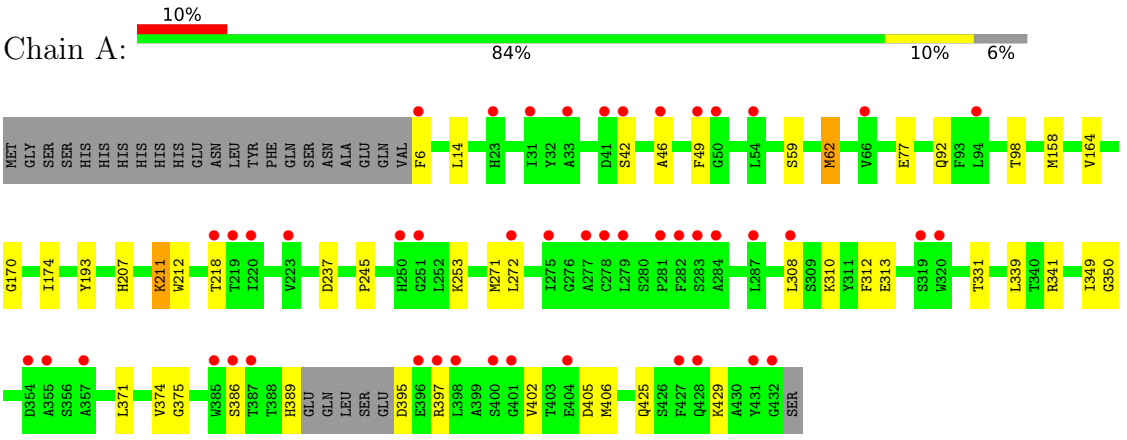
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	187	Total O 187 187	0	0
2	B	161	Total O 161 161	0	0
2	C	216	Total O 216 216	0	0
2	D	215	Total O 215 215	0	0
2	E	200	Total O 200 200	0	0
2	F	219	Total O 220 220	0	1
2	G	168	Total O 168 168	0	0
2	H	190	Total O 190 190	0	0

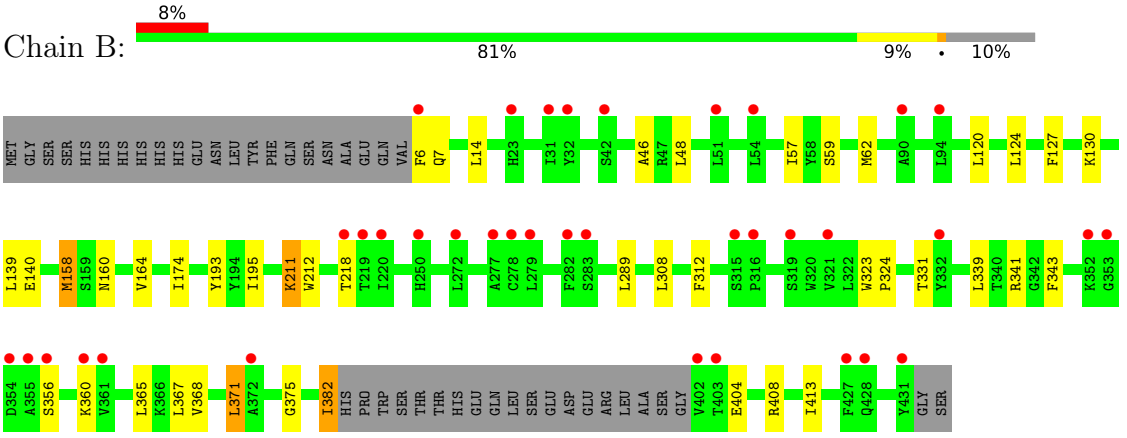
3 Residue-property plots (i)

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.

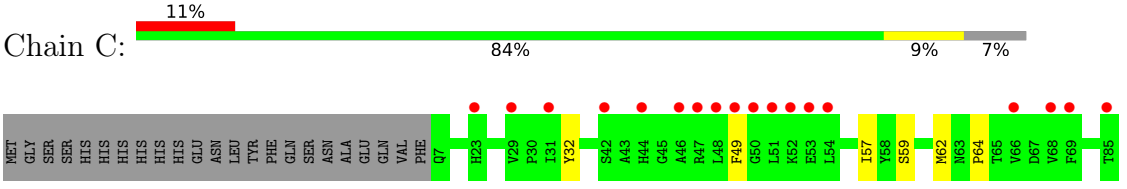
• Molecule 1: Sulfhydrylase FUB7

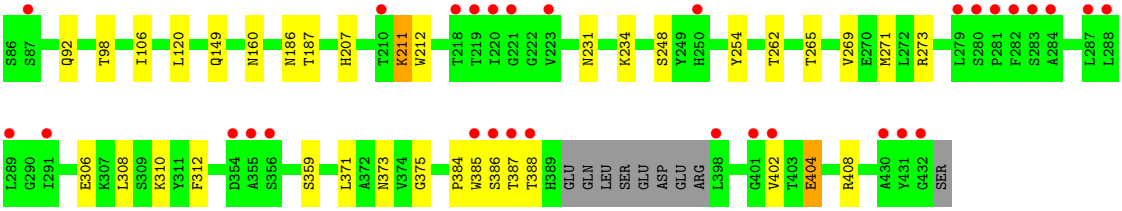


• Molecule 1: Sulfhydrylase FUB7



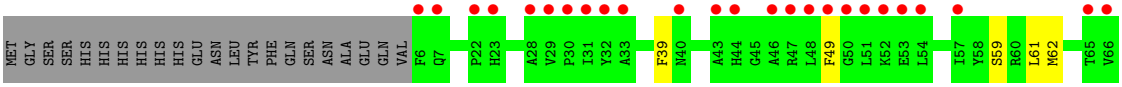
• Molecule 1: Sulfhydrylase FUB7

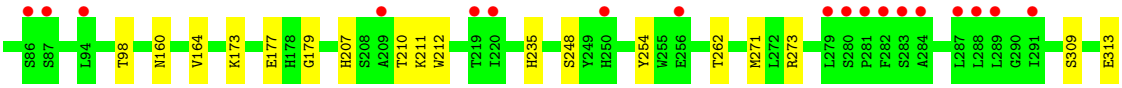


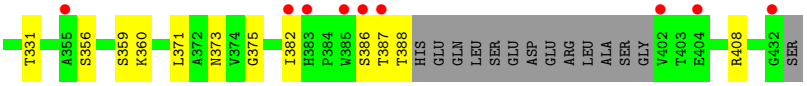


• Molecule 1: Sulfhydrylase FUB7

Chain D:

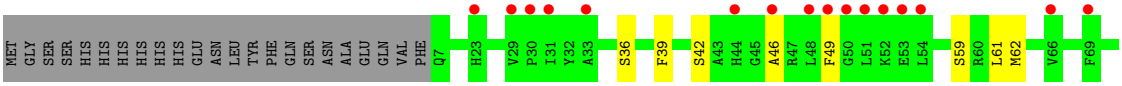


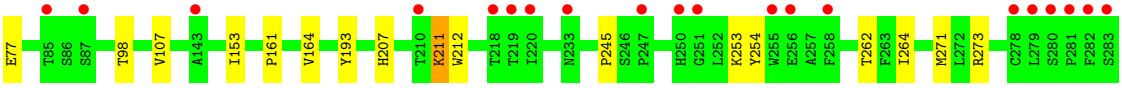


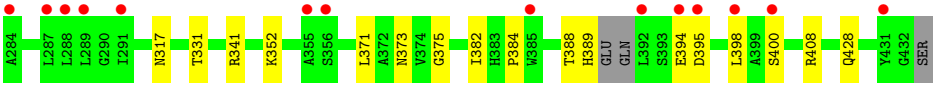


• Molecule 1: Sulfhydrylase FUB7

Chain E:

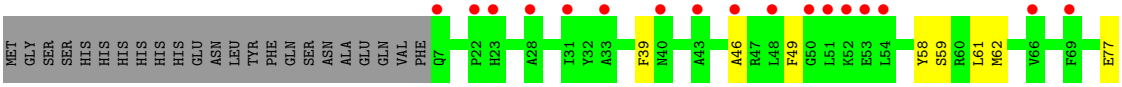


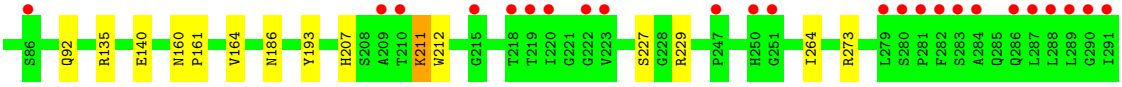


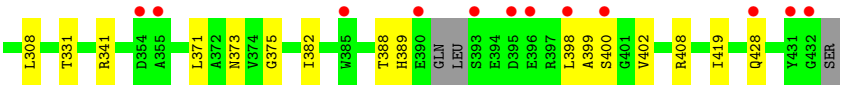


• Molecule 1: Sulfhydrylase FUB7

Chain F:

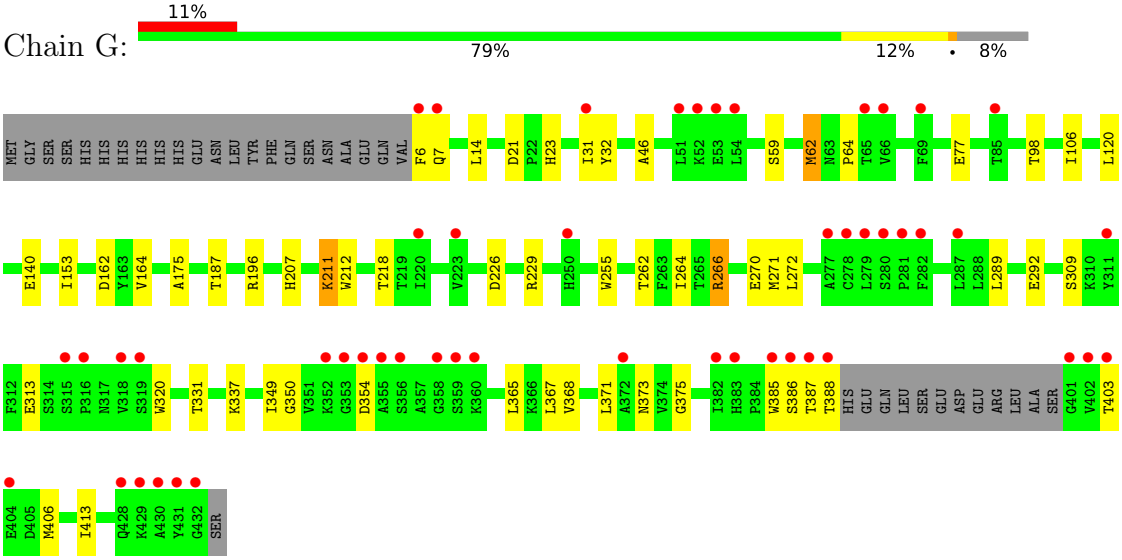






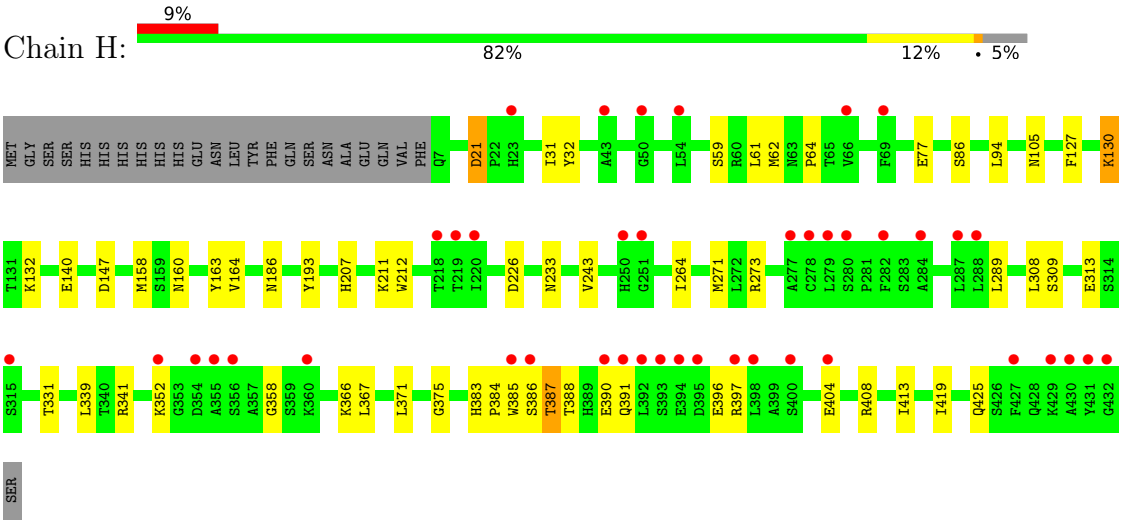
• Molecule 1: Sulfhydrylase FUB7

Chain G:



• Molecule 1: Sulfhydrylase FUB7

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.93Å 195.29Å 112.42Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	47.97 – 1.76 47.97 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.97-1.76) 98.6 (47.97-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.229 0.200 , 0.230	Depositor DCC
R_{free} test set	19975 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27419	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9858e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.47	0/3313	0.62	0/4498
1	B	0.48	0/3192	0.66	1/4332 (0.0%)
1	C	0.51	0/3273	0.66	0/4445
1	D	0.55	0/3251	0.69	1/4415 (0.0%)
1	E	0.46	0/3324	0.63	0/4513
1	F	0.48	0/3325	0.64	0/4514
1	G	0.46	0/3266	0.61	0/4435
1	H	0.45	0/3343	0.64	1/4540 (0.0%)
All	All	0.48	0/26287	0.64	3/35692 (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	E	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	371	LEU	CA-CB-CG	7.04	131.50	115.30
1	D	207	HIS	CB-CA-C	-5.53	99.35	110.40
1	H	130	LYS	CD-CE-NZ	5.24	123.74	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	211	LLP	Mainchain

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	3259	0	3172	29	0
1	B	3143	0	3073	27	0
1	C	3220	0	3140	25	0
1	D	3198	0	3118	19	0
1	E	3271	0	3186	26	0
1	F	3272	0	3180	23	0
1	G	3210	0	3136	40	0
1	H	3289	0	3201	40	0
2	A	187	0	0	0	0
2	B	161	0	0	1	0
2	C	216	0	0	1	0
2	D	215	0	0	0	0
2	E	200	0	0	1	0
2	F	220	0	0	0	0
2	G	168	0	0	2	0
2	H	190	0	0	1	0
All	All	27419	0	25206	206	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 4.

The worst 5 of 206 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:388:THR:HG23	1:E:389:HIS:HD2	1.28	0.98
1:E:388:THR:HG23	1:E:389:HIS:CD2	2.13	0.83
1:D:61:LEU:HD11	1:D:273:ARG:HB2	1.67	0.75
1:G:309:SER:O	1:G:313:GLU:HG2	1.89	0.73
1:C:248:SER:HB3	1:C:273:ARG:HH12	1.58	0.67

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	417/450 (93%)	406 (97%)	11 (3%)	0	100	100
1	B	402/450 (89%)	393 (98%)	9 (2%)	0	100	100
1	C	413/450 (92%)	405 (98%)	8 (2%)	0	100	100
1	D	409/450 (91%)	400 (98%)	9 (2%)	0	100	100
1	E	419/450 (93%)	405 (97%)	14 (3%)	0	100	100
1	F	419/450 (93%)	408 (97%)	11 (3%)	0	100	100
1	G	411/450 (91%)	405 (98%)	6 (2%)	0	100	100
1	H	423/450 (94%)	414 (98%)	9 (2%)	0	100	100
All	All	3313/3600 (92%)	3236 (98%)	77 (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	339/365 (93%)	336 (99%)	3 (1%)	78	67
1	B	327/365 (90%)	321 (98%)	6 (2%)	59	40
1	C	335/365 (92%)	332 (99%)	3 (1%)	78	67
1	D	333/365 (91%)	331 (99%)	2 (1%)	86	79
1	E	341/365 (93%)	338 (99%)	3 (1%)	78	67
1	F	341/365 (93%)	340 (100%)	1 (0%)	92	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	334/365 (92%)	328 (98%)	6 (2%)	59 40
1	H	343/365 (94%)	337 (98%)	6 (2%)	60 42
All	All	2693/2920 (92%)	2663 (99%)	30 (1%)	73 60

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	394	GLU
1	H	387	THR
1	F	428	GLN
1	H	396	GLU
1	H	21	ASP

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

Mol	Chain	Res	Type
1	E	389	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	A	211	1	23,24,25	1.98	5 (21%)	25,32,34	1.39	5 (20%)
1	LLP	H	211	1	23,24,25	1.78	5 (21%)	25,32,34	1.56	6 (24%)
1	LLP	E	211	1	23,24,25	1.57	4 (17%)	25,32,34	1.57	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	F	211	1	23,24,25	1.84	5 (21%)	25,32,34	1.45	4 (16%)
1	LLP	G	211	1	23,24,25	2.06	6 (26%)	25,32,34	1.41	4 (16%)
1	LLP	B	211	1	23,24,25	2.04	6 (26%)	25,32,34	1.42	5 (20%)
1	LLP	D	211	1	23,24,25	1.84	6 (26%)	25,32,34	1.39	4 (16%)
1	LLP	C	211	1	23,24,25	2.19	8 (34%)	25,32,34	1.46	5 (20%)

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	A	211	1	-	4/16/17/19	0/1/1/1
1	LLP	H	211	1	-	4/16/17/19	0/1/1/1
1	LLP	E	211	1	-	4/16/17/19	0/1/1/1
1	LLP	F	211	1	-	4/16/17/19	0/1/1/1
1	LLP	G	211	1	-	4/16/17/19	0/1/1/1
1	LLP	B	211	1	-	5/16/17/19	0/1/1/1
1	LLP	D	211	1	-	4/16/17/19	0/1/1/1
1	LLP	C	211	1	-	4/16/17/19	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	211	LLP	P-OP4	6.08	1.79	1.60
1	A	211	LLP	P-OP4	5.91	1.79	1.60
1	B	211	LLP	P-OP4	5.55	1.78	1.60
1	C	211	LLP	CB-CA	5.21	1.60	1.53
1	H	211	LLP	P-OP4	4.95	1.76	1.60

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	211	LLP	OP4-P-OP1	-4.42	94.07	106.47
1	C	211	LLP	OP3-P-OP2	3.45	120.83	107.64
1	D	211	LLP	OP4-P-OP1	-3.32	97.16	106.47
1	F	211	LLP	OP4-P-OP1	-3.30	97.21	106.47
1	H	211	LLP	OP3-P-OP2	3.19	119.84	107.64

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	211	LLP	O-C-CA-CB
1	C	211	LLP	O-C-CA-CB
1	D	211	LLP	O-C-CA-CB
1	E	211	LLP	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	211	LLP	2	0
1	F	211	LLP	1	0
1	G	211	LLP	1	0
1	B	211	LLP	1	0
1	C	211	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	421/450 (93%)	0.53	47 (11%) 5 7	23, 35, 59, 76	1 (0%)
1	B	406/450 (90%)	0.54	37 (9%) 9 11	23, 35, 59, 74	1 (0%)
1	C	417/450 (92%)	0.47	49 (11%) 4 6	20, 30, 57, 72	1 (0%)
1	D	413/450 (91%)	0.47	52 (12%) 3 5	20, 30, 53, 75	1 (0%)
1	E	423/450 (94%)	0.56	50 (11%) 4 6	20, 33, 56, 77	1 (0%)
1	F	423/450 (94%)	0.50	53 (12%) 3 5	21, 32, 54, 69	2 (0%)
1	G	414/450 (92%)	0.60	50 (12%) 4 6	23, 36, 61, 75	1 (0%)
1	H	425/450 (94%)	0.56	42 (9%) 7 10	23, 35, 60, 77	1 (0%)
All	All	3342/3600 (92%)	0.53	380 (11%) 5 7	20, 33, 58, 77	9 (0%)

The worst 5 of 380 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	385	TRP	9.5
1	E	54	LEU	7.3
1	A	385	TRP	6.5
1	C	385	TRP	6.5
1	D	6	PHE	6.1

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

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	A	211	24/25	0.97	0.11	25,29,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	B	211	24/25	0.97	0.10	24,29,33,37	0
1	LLP	C	211	24/25	0.97	0.12	19,25,31,33	0
1	LLP	D	211	24/25	0.97	0.13	19,24,30,32	0
1	LLP	E	211	24/25	0.97	0.13	23,27,31,34	0
1	LLP	G	211	24/25	0.97	0.12	23,32,34,38	0
1	LLP	F	211	24/25	0.98	0.15	23,27,31,34	0
1	LLP	H	211	24/25	0.98	0.12	23,31,36,37	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.