wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2016 – 05:45 PM EDT

PDB ID	:	5ECP
Title	:	Crystal Structure of FIN219-FIP1 complex with JA, MET and ATP
Authors	:	Chen, C.Y.; Cheng, Y.S.
Deposited on	:	2015-10-20
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

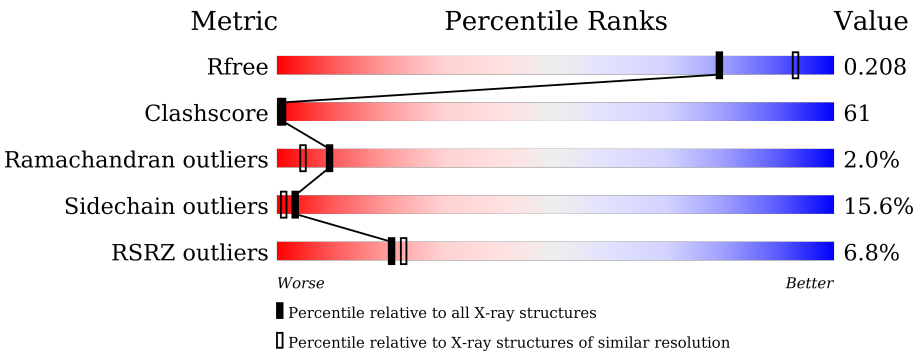
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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	575	8% 23% 61% 13% ••
1	D	575	10% 23% 60% 15% ••
2	B	223	4% 35% 54% 6% • •
2	C	223	% 30% 56% 9% •
2	E	223	6% 35% 53% 8% •
2	F	223	% 25% 58% 13% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ATP	A	603	-	-	X	-
5	ATP	D	603	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17707 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 Jasmonic acid-amido synthetase JAR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	569	4479	2859	748	850	22	0	0	0
1	D	569	4479	2859	748	850	22	0	0	0

- Molecule 2 is a protein called Glutathione S-transferase U20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1748	1136	284	323	5	0	0	0
2	C	214	1748	1136	284	323	5	0	0	0
2	E	214	1748	1136	284	323	5	0	0	0
2	F	214	1748	1136	284	323	5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q8L7C9
B	-4	HIS	-	expression tag	UNP Q8L7C9
B	-3	HIS	-	expression tag	UNP Q8L7C9
B	-2	HIS	-	expression tag	UNP Q8L7C9
B	-1	HIS	-	expression tag	UNP Q8L7C9
B	0	HIS	-	expression tag	UNP Q8L7C9
C	-5	HIS	-	expression tag	UNP Q8L7C9
C	-4	HIS	-	expression tag	UNP Q8L7C9
C	-3	HIS	-	expression tag	UNP Q8L7C9
C	-2	HIS	-	expression tag	UNP Q8L7C9
C	-1	HIS	-	expression tag	UNP Q8L7C9
C	0	HIS	-	expression tag	UNP Q8L7C9

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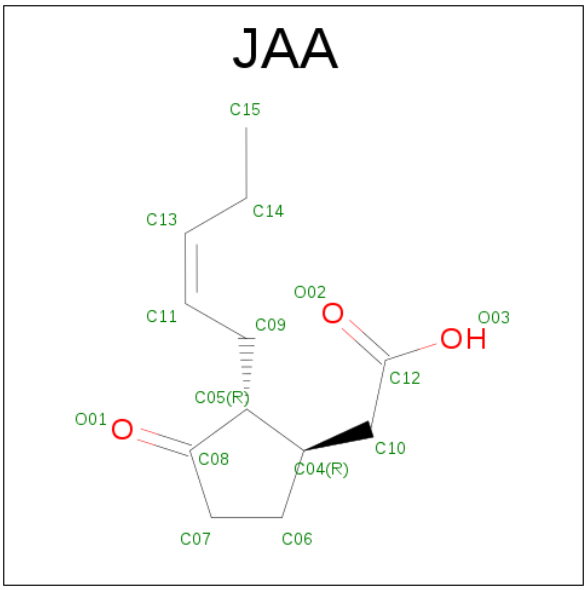
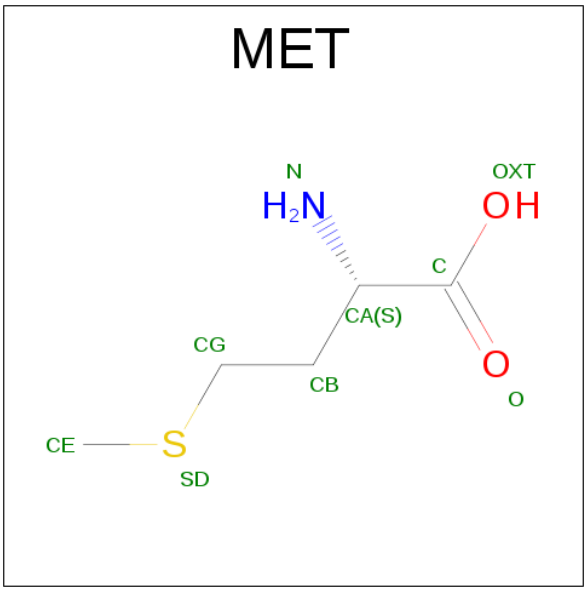
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	expression tag	UNP Q8L7C9
E	-4	HIS	-	expression tag	UNP Q8L7C9
E	-3	HIS	-	expression tag	UNP Q8L7C9
E	-2	HIS	-	expression tag	UNP Q8L7C9
E	-1	HIS	-	expression tag	UNP Q8L7C9
E	0	HIS	-	expression tag	UNP Q8L7C9
F	-5	HIS	-	expression tag	UNP Q8L7C9
F	-4	HIS	-	expression tag	UNP Q8L7C9
F	-3	HIS	-	expression tag	UNP Q8L7C9
F	-2	HIS	-	expression tag	UNP Q8L7C9
F	-1	HIS	-	expression tag	UNP Q8L7C9
F	0	HIS	-	expression tag	UNP Q8L7C9

- Molecule 3 is {(1R,2R)-3-oxo-2-[(2Z)-pent-2-en-1-yl]cyclopentyl}acetic acid (three-letter code: JAA) (formula: $C_{12}H_{18}O_3$).



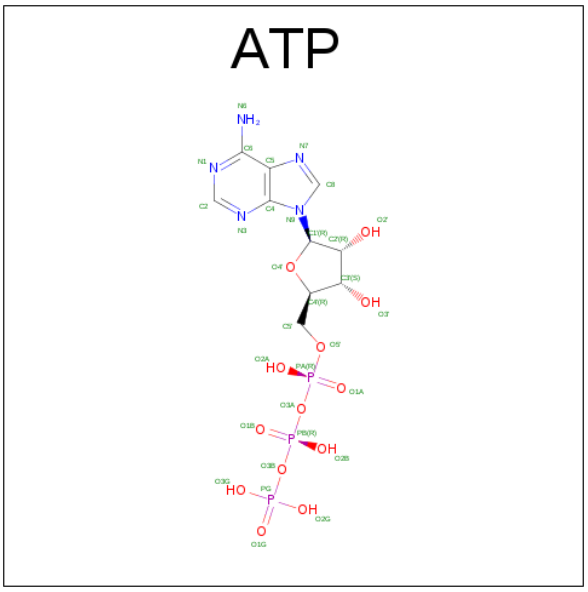
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	15	12	3	0	0
			Total	C	O		
3	D	1	15	12	3	0	0

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	9	5	1	2	1	0	0
			Total	C	N	O	S		
4	D	1	9	5	1	2	1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0

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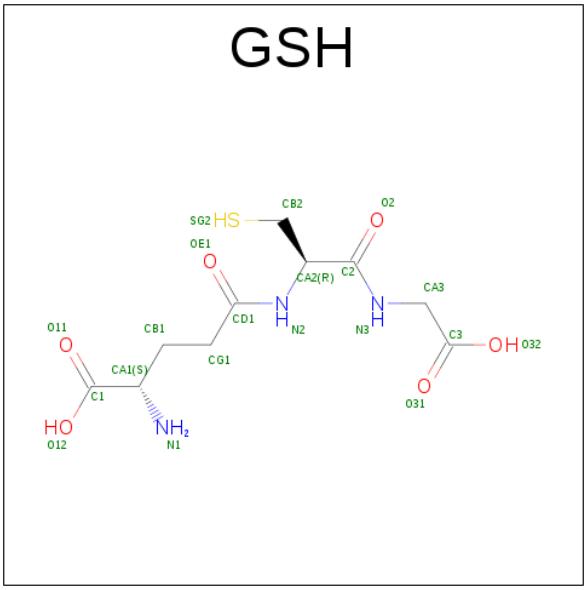
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	D	1	31	10	5	13	3	0	0

- Molecule 6 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	20	10	3	6	1	0	0
			Total	C	N	O	S		
6	C	1	20	10	3	6	1	0	0
			Total	C	N	O	S		
6	E	1	20	10	3	6	1	0	0
			Total	C	N	O	S		
6	F	1	20	10	3	6	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	357	357	357	0	0
			Total	O		
7	B	193	193	193	0	0
			Total	O		
7	C	214	214	214	0	0
			Total	O		
7	D	403	403	403	0	0

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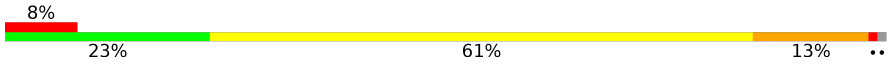
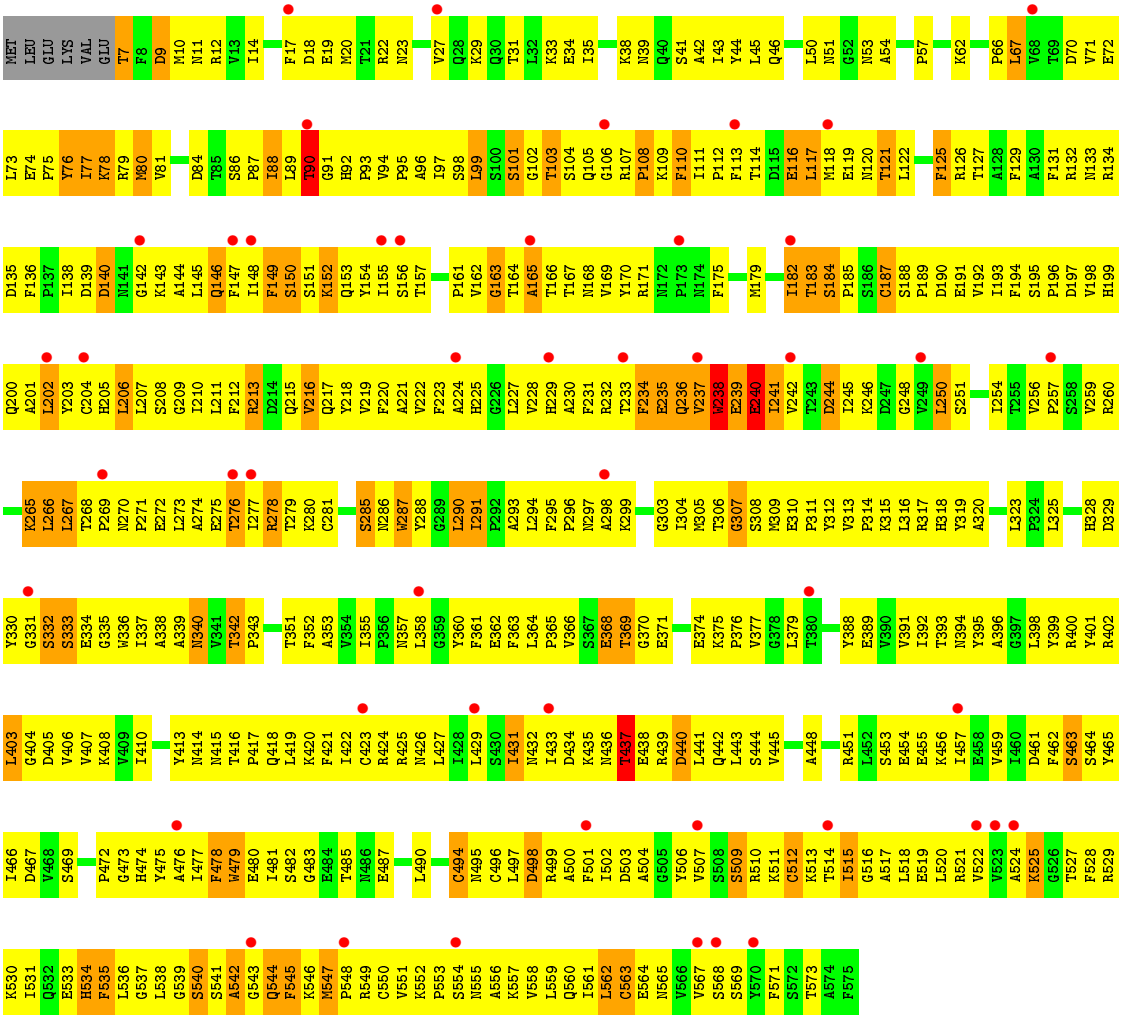
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	E	201	201	201	0	0
			Total	O		
7	F	199	199	199	0	0

3 Residue-property plots (i)

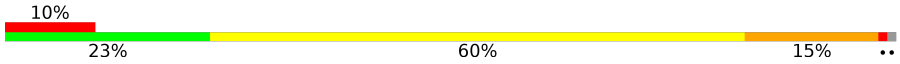
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

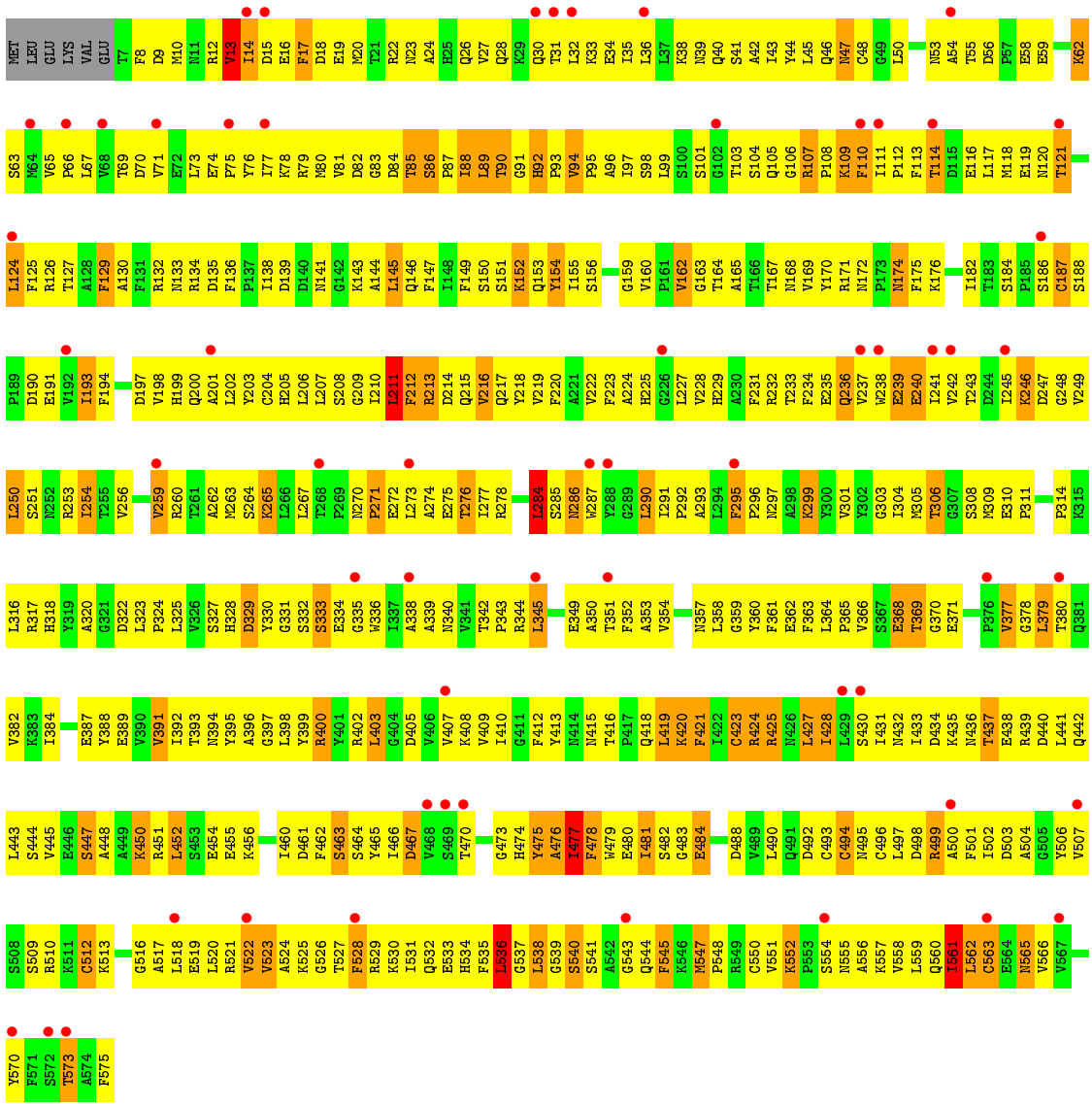
- Molecule 1: Jasmonic acid-amido synthetase JAR1

Chain A: 



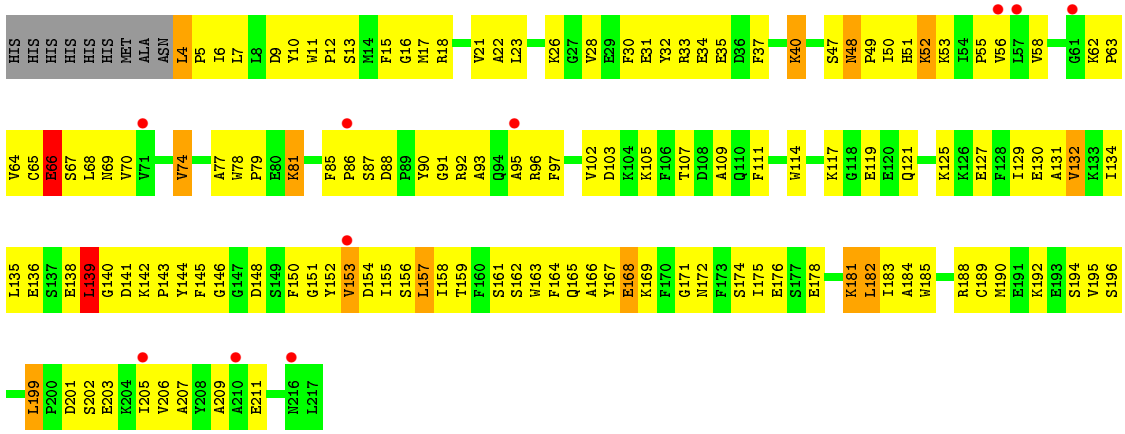
- Molecule 1: Jasmonic acid-amido synthetase JAR1

Chain D: 



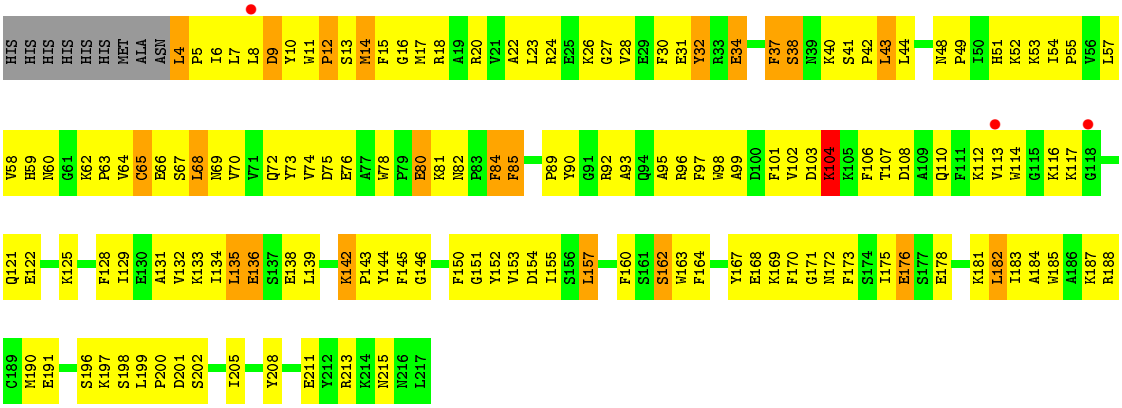
- Molecule 2: Glutathione S-transferase U20

Chain B:



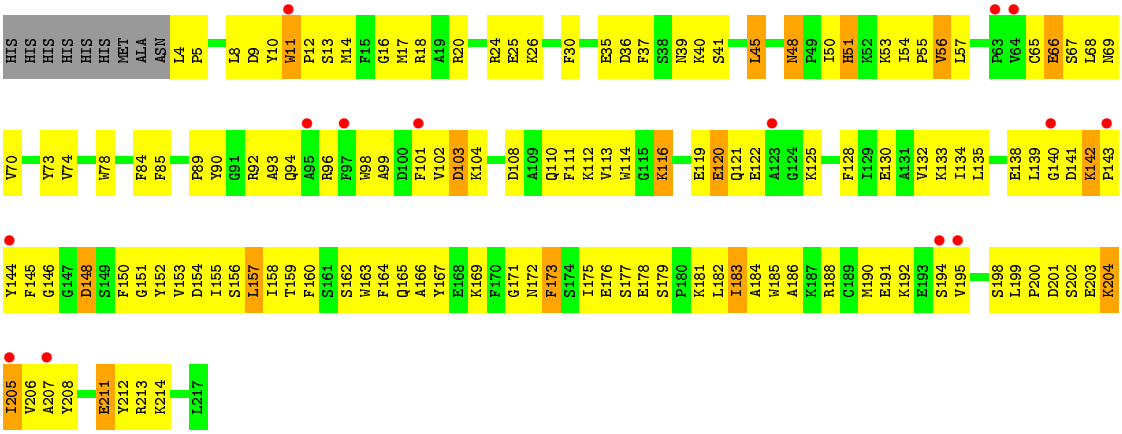
- Molecule 2: Glutathione S-transferase U20

Chain C:



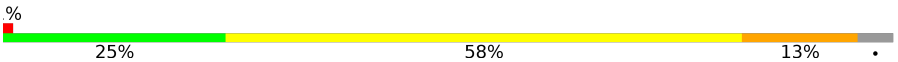
- Molecule 2: Glutathione S-transferase U20

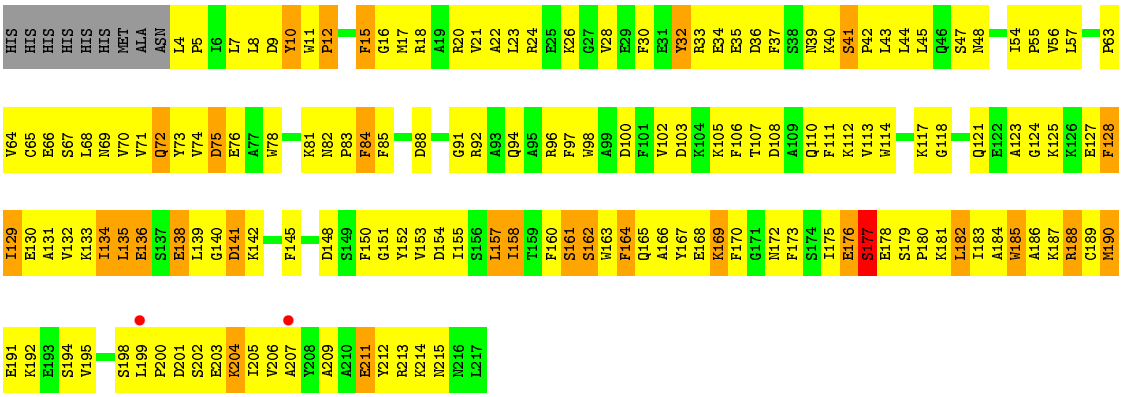
Chain E:



- Molecule 2: Glutathione S-transferase U20

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.71Å 53.70Å 192.03Å 89.96° 90.16° 113.24°	Depositor
Resolution (Å)	23.35 – 2.25 23.35 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.5 (23.35-2.25) 95.1 (23.35-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692+SVN)	Depositor
R, R_{free}	0.185 , 0.208 0.185 , 0.208	Depositor DCC
R_{free} test set	2256 reflections (2.53%)	DCC
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 247.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l 0.076 for -k,-h,-l 0.076 for k,h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	17707	wwPDB-VP
Average B, all atoms (Å^2)	11.0	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 27.70 % 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 2.1005e-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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, ATP, JAA

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	0.67	1/4581 (0.0%)	0.82	6/6219 (0.1%)
1	D	0.66	0/4581	0.80	7/6219 (0.1%)
2	B	0.72	0/1799	0.70	1/2428 (0.0%)
2	C	0.84	0/1799	0.72	0/2428
2	E	0.73	0/1799	0.69	1/2428 (0.0%)
2	F	0.90	0/1799	0.85	1/2428 (0.0%)
All	All	0.73	1/16358 (0.0%)	0.78	16/22150 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	TRP	CB-CG	-5.44	1.40	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	LEU	CA-CB-CG	7.91	133.50	115.30
1	A	99	LEU	CB-CG-CD2	6.70	122.38	111.00
1	A	290	LEU	CB-CG-CD1	-6.05	100.72	111.00
1	A	99	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	D	536	LEU	CA-CB-CG	5.85	128.76	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4479	0	4434	615	6
1	D	4479	0	4434	639	5
2	B	1748	0	1704	187	1
2	C	1748	0	1704	197	1
2	E	1748	0	1704	180	1
2	F	1748	0	1704	211	1
3	A	15	0	0	0	0
3	D	15	0	0	3	0
4	A	9	0	8	2	0
4	D	9	0	8	5	0
5	A	31	0	8	17	0
5	D	31	0	8	26	0
6	B	20	0	15	1	0
6	C	20	0	15	0	0
6	E	20	0	15	3	0
6	F	20	0	15	0	0
7	A	357	0	0	75	7
7	B	193	0	0	28	2
7	C	214	0	0	30	1
7	D	403	0	0	74	4
7	E	201	0	0	28	1
7	F	199	0	0	35	3
All	All	17707	0	15776	1939	22

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 61.

The worst 5 of 1939 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:A:121:THR:HG21	1:A:175:PHE:CE1	1.69	1.27
1:A:121:THR:CG2	1:A:175:PHE:HE1	1.56	1.18
1:A:120:ASN:HD21	1:A:358:LEU:HD22	1.17	1.10
1:A:121:THR:HG21	1:A:175:PHE:HE1	0.93	1.05
1:D:334:GLU:O	1:D:394:ASN:ND2	1.93	1.02

The worst 5 of 22 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ASN:ND2	1:D:435:LYS:O[1_655]	1.96	0.24
7:F:552:HOH:O	7:F:577:HOH:O[1_665]	2.00	0.20
1:A:239:GLU:OE1	2:F:178:GLU:N[1_554]	2.01	0.19
7:D:989:HOH:O	7:D:1008:HOH:O[1_665]	2.04	0.16
7:D:936:HOH:O	7:D:988:HOH:O[1_655]	2.04	0.16

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	567/575 (99%)	514 (91%)	38 (7%)	15 (3%)	7	3
1	D	567/575 (99%)	516 (91%)	36 (6%)	15 (3%)	7	3
2	B	212/223 (95%)	200 (94%)	10 (5%)	2 (1%)	21	18
2	C	212/223 (95%)	198 (93%)	12 (6%)	2 (1%)	21	18
2	E	212/223 (95%)	199 (94%)	12 (6%)	1 (0%)	34	34
2	F	212/223 (95%)	196 (92%)	11 (5%)	5 (2%)	7	3
All	All	1982/2042 (97%)	1823 (92%)	119 (6%)	40 (2%)	9	5

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	TRP
1	A	241	ILE
1	A	368	GLU
1	A	540	SER
1	A	542	ALA

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	499/505 (99%)	425 (85%)	74 (15%)	4 2
1	D	499/505 (99%)	402 (81%)	97 (19%)	2 0
2	B	187/195 (96%)	171 (91%)	16 (9%)	13 11
2	C	187/195 (96%)	164 (88%)	23 (12%)	6 4
2	E	187/195 (96%)	161 (86%)	26 (14%)	4 2
2	F	187/195 (96%)	150 (80%)	37 (20%)	1 0
All	All	1746/1790 (98%)	1473 (84%)	273 (16%)	3 1

5 of 273 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	89	LEU
1	D	251	SER
2	F	133	LYS
1	D	107	ARG
1	D	162	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	39	ASN
1	D	495	ASN
2	E	121	GLN
1	D	28	GLN

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Mol	Chain	Res	Type
2	E	172	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 ligands 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	$\#\|Z\| > 2$
3	JAA	A	601	-	12,15,15	5.80	6 (50%)	12,19,19	2.67	6 (50%)
4	MET	A	602	-	5,8,8	0.66	0	3,9,9	0.69	0
5	ATP	A	603	-	26,33,33	4.57	14 (53%)	26,52,52	2.70	12 (46%)
6	GSH	B	301	-	13,19,19	1.97	5 (38%)	15,24,24	3.26	7 (46%)
6	GSH	C	301	-	13,19,19	1.66	4 (30%)	15,24,24	3.20	6 (40%)
3	JAA	D	601	-	12,15,15	5.72	6 (50%)	12,19,19	2.76	6 (50%)
4	MET	D	602	-	5,8,8	0.34	0	3,9,9	0.19	0
5	ATP	D	603	-	26,33,33	4.86	14 (53%)	26,52,52	3.34	10 (38%)
6	GSH	E	301	-	13,19,19	1.71	3 (23%)	15,24,24	3.24	8 (53%)
6	GSH	F	301	-	13,19,19	1.67	4 (30%)	15,24,24	4.17	7 (46%)

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
3	JAA	A	601	-	-	0/7/22/22	0/1/1/1
4	MET	A	602	-	-	0/4/8/8	0/0/0/0
5	ATP	A	603	-	-	0/18/38/38	0/3/3/3
6	GSH	B	301	-	-	0/18/24/24	0/0/0/0
6	GSH	C	301	-	-	0/18/24/24	0/0/0/0
3	JAA	D	601	-	-	0/7/22/22	0/1/1/1
4	MET	D	602	-	-	0/4/8/8	0/0/0/0
5	ATP	D	603	-	-	0/18/38/38	0/3/3/3
6	GSH	E	301	-	-	0/18/24/24	0/0/0/0
6	GSH	F	301	-	-	0/18/24/24	0/0/0/0

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JAA	C05-C08	-13.71	1.29	1.52
3	D	601	JAA	C05-C08	-13.45	1.30	1.52
3	D	601	JAA	C06-C04	-10.67	1.25	1.53
5	D	603	ATP	C2'-C1'	-10.56	1.36	1.53
3	A	601	JAA	C06-C04	-10.30	1.26	1.53

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	301	GSH	CA2-CB2-SG2	-13.98	98.63	113.99
6	B	301	GSH	CA2-CB2-SG2	-10.45	102.51	113.99
6	E	301	GSH	CA2-CB2-SG2	-10.26	102.72	113.99
6	C	301	GSH	CA2-CB2-SG2	-9.78	103.25	113.99
5	D	603	ATP	C4'-O4'-C1'	-9.63	99.43	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	MET	2	0
5	A	603	ATP	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	301	GSH	1	0
3	D	601	JAA	3	0
4	D	602	MET	5	0
5	D	603	ATP	26	0
6	E	301	GSH	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	569/575 (98%)	0.68	48 (8%) 14 15	3, 14, 22, 28	0
1	D	569/575 (98%)	0.79	58 (10%) 9 9	3, 15, 24, 31	0
2	B	214/223 (95%)	0.45	10 (4%) 35 39	4, 11, 20, 28	0
2	C	214/223 (95%)	0.20	3 (1%) 78 80	2, 3, 7, 11	0
2	E	214/223 (95%)	0.43	14 (6%) 22 24	4, 9, 16, 27	0
2	F	214/223 (95%)	0.16	2 (0%) 85 87	2, 3, 7, 11	0
All	All	1994/2042 (97%)	0.55	135 (6%) 20 23	2, 12, 22, 31	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	95	ALA	4.6
1	A	113	PHE	4.0
1	A	554	SER	3.9
2	B	205	ILE	3.6
1	D	111	ILE	3.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å^2)	Q<0.9
3	JAA	D	601	15/15	0.88	0.23	1.03	12,19,30,35	0
6	GSH	F	301	20/20	0.91	0.19	0.86	9,16,23,25	0
4	MET	D	602	9/9	0.90	0.19	0.61	14,20,29,39	0
3	JAA	A	601	15/15	0.88	0.21	0.31	12,19,24,28	0
5	ATP	D	603	31/31	0.92	0.18	-0.08	13,20,30,32	0
4	MET	A	602	9/9	0.93	0.18	-0.37	14,20,24,26	0
6	GSH	E	301	20/20	0.92	0.15	-0.42	6,13,21,22	0
6	GSH	C	301	20/20	0.93	0.14	-0.44	5,9,17,20	0
5	ATP	A	603	31/31	0.94	0.15	-0.99	8,19,26,28	0
6	GSH	B	301	20/20	0.94	0.12	-1.22	3,5,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.