wwPDB X-ray Structure Validation Summary Report (i)

Apr 11, 2016 – 03:38 PM EDT

PDB ID	:	4ZWQ
Title	:	Crystal Structure of the Bacteriophage T4 recombination mediator protein UvsY, Lattice Type I
Authors	:	Gajewski, S.; White, S.W.
Deposited on	:	2015-05-19
Resolution	:	2.35 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:

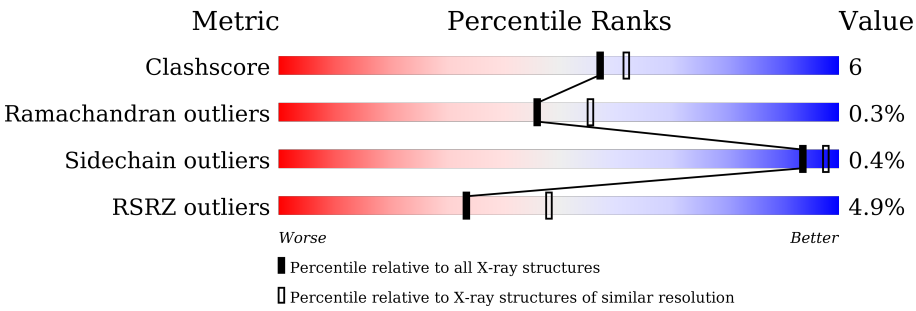
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.35 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))
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	157	7%, 71%, 15%, 13%
1	B	157	%, 68%, 18%, 14%
1	C	157	%, 70%, 15%, 15%
1	D	157	%, 74%, 12%, 14%
1	E	157	%, 73%, 13%, 14%
1	F	157	2%, 73%, 13%, 15%
1	G	157	17%, 74%, 10%, 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7494 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 Recombination protein uvsY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	136	1084	687	184	206	7	0	0	0
			Total	C	N	O	S			
1	B	135	1083	689	185	202	7	0	0	0
			Total	C	N	O	S			
1	C	134	1072	681	181	204	6	0	0	0
			Total	C	N	O	S			
1	D	135	1084	689	183	205	7	0	0	0
			Total	C	N	O	S			
1	E	135	1077	686	183	201	7	0	0	0
			Total	C	N	O	S			
1	F	134	1068	678	180	204	6	0	0	0
			Total	C	N	O	S			
1	G	132	1026	649	174	198	5	0	0	0

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P04537
A	-18	GLY	-	expression tag	UNP P04537
A	-17	SER	-	expression tag	UNP P04537
A	-16	SER	-	expression tag	UNP P04537
A	-15	HIS	-	expression tag	UNP P04537
A	-14	HIS	-	expression tag	UNP P04537
A	-13	HIS	-	expression tag	UNP P04537
A	-12	HIS	-	expression tag	UNP P04537
A	-11	HIS	-	expression tag	UNP P04537
A	-10	HIS	-	expression tag	UNP P04537
A	-9	SER	-	expression tag	UNP P04537
A	-8	SER	-	expression tag	UNP P04537
A	-7	GLY	-	expression tag	UNP P04537
A	-6	LEU	-	expression tag	UNP P04537
A	-5	VAL	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	expression tag	UNP P04537
A	-3	ARG	-	expression tag	UNP P04537
A	-2	GLY	-	expression tag	UNP P04537
A	-1	SER	-	expression tag	UNP P04537
A	0	HIS	-	expression tag	UNP P04537
B	-19	MET	-	expression tag	UNP P04537
B	-18	GLY	-	expression tag	UNP P04537
B	-17	SER	-	expression tag	UNP P04537
B	-16	SER	-	expression tag	UNP P04537
B	-15	HIS	-	expression tag	UNP P04537
B	-14	HIS	-	expression tag	UNP P04537
B	-13	HIS	-	expression tag	UNP P04537
B	-12	HIS	-	expression tag	UNP P04537
B	-11	HIS	-	expression tag	UNP P04537
B	-10	HIS	-	expression tag	UNP P04537
B	-9	SER	-	expression tag	UNP P04537
B	-8	SER	-	expression tag	UNP P04537
B	-7	GLY	-	expression tag	UNP P04537
B	-6	LEU	-	expression tag	UNP P04537
B	-5	VAL	-	expression tag	UNP P04537
B	-4	PRO	-	expression tag	UNP P04537
B	-3	ARG	-	expression tag	UNP P04537
B	-2	GLY	-	expression tag	UNP P04537
B	-1	SER	-	expression tag	UNP P04537
B	0	HIS	-	expression tag	UNP P04537
C	-19	MET	-	expression tag	UNP P04537
C	-18	GLY	-	expression tag	UNP P04537
C	-17	SER	-	expression tag	UNP P04537
C	-16	SER	-	expression tag	UNP P04537
C	-15	HIS	-	expression tag	UNP P04537
C	-14	HIS	-	expression tag	UNP P04537
C	-13	HIS	-	expression tag	UNP P04537
C	-12	HIS	-	expression tag	UNP P04537
C	-11	HIS	-	expression tag	UNP P04537
C	-10	HIS	-	expression tag	UNP P04537
C	-9	SER	-	expression tag	UNP P04537
C	-8	SER	-	expression tag	UNP P04537
C	-7	GLY	-	expression tag	UNP P04537
C	-6	LEU	-	expression tag	UNP P04537
C	-5	VAL	-	expression tag	UNP P04537
C	-4	PRO	-	expression tag	UNP P04537
C	-3	ARG	-	expression tag	UNP P04537

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04537
C	-1	SER	-	expression tag	UNP P04537
C	0	HIS	-	expression tag	UNP P04537
D	-19	MET	-	expression tag	UNP P04537
D	-18	GLY	-	expression tag	UNP P04537
D	-17	SER	-	expression tag	UNP P04537
D	-16	SER	-	expression tag	UNP P04537
D	-15	HIS	-	expression tag	UNP P04537
D	-14	HIS	-	expression tag	UNP P04537
D	-13	HIS	-	expression tag	UNP P04537
D	-12	HIS	-	expression tag	UNP P04537
D	-11	HIS	-	expression tag	UNP P04537
D	-10	HIS	-	expression tag	UNP P04537
D	-9	SER	-	expression tag	UNP P04537
D	-8	SER	-	expression tag	UNP P04537
D	-7	GLY	-	expression tag	UNP P04537
D	-6	LEU	-	expression tag	UNP P04537
D	-5	VAL	-	expression tag	UNP P04537
D	-4	PRO	-	expression tag	UNP P04537
D	-3	ARG	-	expression tag	UNP P04537
D	-2	GLY	-	expression tag	UNP P04537
D	-1	SER	-	expression tag	UNP P04537
D	0	HIS	-	expression tag	UNP P04537
E	-19	MET	-	expression tag	UNP P04537
E	-18	GLY	-	expression tag	UNP P04537
E	-17	SER	-	expression tag	UNP P04537
E	-16	SER	-	expression tag	UNP P04537
E	-15	HIS	-	expression tag	UNP P04537
E	-14	HIS	-	expression tag	UNP P04537
E	-13	HIS	-	expression tag	UNP P04537
E	-12	HIS	-	expression tag	UNP P04537
E	-11	HIS	-	expression tag	UNP P04537
E	-10	HIS	-	expression tag	UNP P04537
E	-9	SER	-	expression tag	UNP P04537
E	-8	SER	-	expression tag	UNP P04537
E	-7	GLY	-	expression tag	UNP P04537
E	-6	LEU	-	expression tag	UNP P04537
E	-5	VAL	-	expression tag	UNP P04537
E	-4	PRO	-	expression tag	UNP P04537
E	-3	ARG	-	expression tag	UNP P04537
E	-2	GLY	-	expression tag	UNP P04537
E	-1	SER	-	expression tag	UNP P04537

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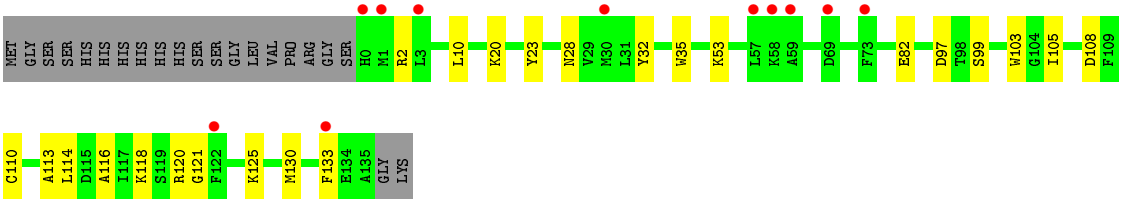
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P04537
F	-19	MET	-	expression tag	UNP P04537
F	-18	GLY	-	expression tag	UNP P04537
F	-17	SER	-	expression tag	UNP P04537
F	-16	SER	-	expression tag	UNP P04537
F	-15	HIS	-	expression tag	UNP P04537
F	-14	HIS	-	expression tag	UNP P04537
F	-13	HIS	-	expression tag	UNP P04537
F	-12	HIS	-	expression tag	UNP P04537
F	-11	HIS	-	expression tag	UNP P04537
F	-10	HIS	-	expression tag	UNP P04537
F	-9	SER	-	expression tag	UNP P04537
F	-8	SER	-	expression tag	UNP P04537
F	-7	GLY	-	expression tag	UNP P04537
F	-6	LEU	-	expression tag	UNP P04537
F	-5	VAL	-	expression tag	UNP P04537
F	-4	PRO	-	expression tag	UNP P04537
F	-3	ARG	-	expression tag	UNP P04537
F	-2	GLY	-	expression tag	UNP P04537
F	-1	SER	-	expression tag	UNP P04537
F	0	HIS	-	expression tag	UNP P04537
G	-19	MET	-	expression tag	UNP P04537
G	-18	GLY	-	expression tag	UNP P04537
G	-17	SER	-	expression tag	UNP P04537
G	-16	SER	-	expression tag	UNP P04537
G	-15	HIS	-	expression tag	UNP P04537
G	-14	HIS	-	expression tag	UNP P04537
G	-13	HIS	-	expression tag	UNP P04537
G	-12	HIS	-	expression tag	UNP P04537
G	-11	HIS	-	expression tag	UNP P04537
G	-10	HIS	-	expression tag	UNP P04537
G	-9	SER	-	expression tag	UNP P04537
G	-8	SER	-	expression tag	UNP P04537
G	-7	GLY	-	expression tag	UNP P04537
G	-6	LEU	-	expression tag	UNP P04537
G	-5	VAL	-	expression tag	UNP P04537
G	-4	PRO	-	expression tag	UNP P04537
G	-3	ARG	-	expression tag	UNP P04537
G	-2	GLY	-	expression tag	UNP P04537
G	-1	SER	-	expression tag	UNP P04537
G	0	HIS	-	expression tag	UNP P04537

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.

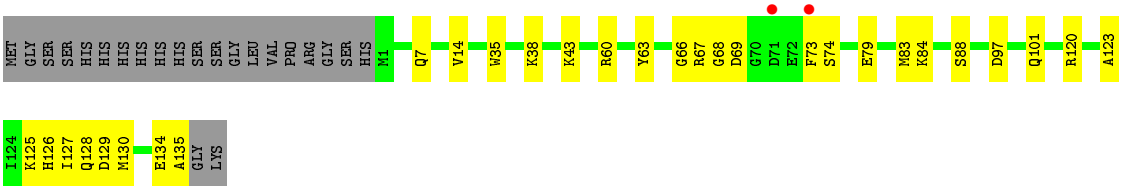
- Molecule 1: Recombination protein uvsY

Chain A:



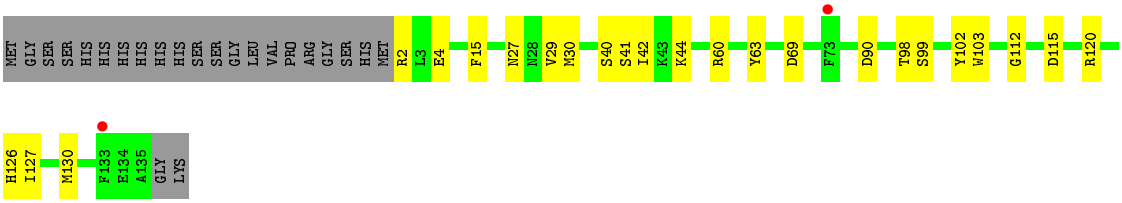
- Molecule 1: Recombination protein uvsY

Chain B:



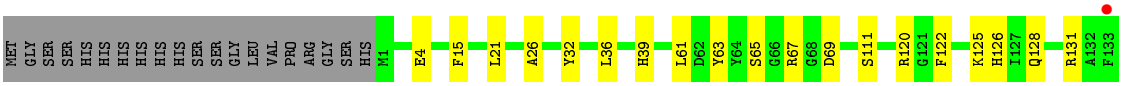
- Molecule 1: Recombination protein uvsY

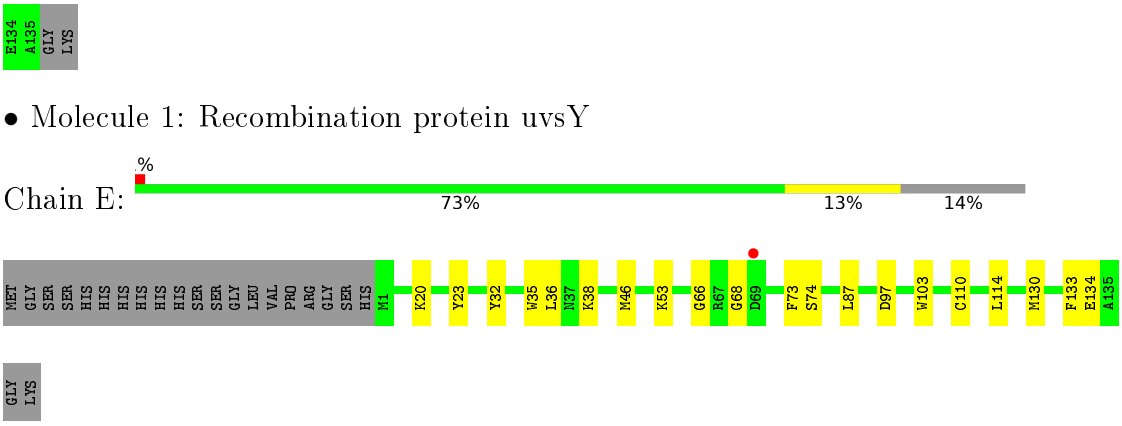
Chain C:

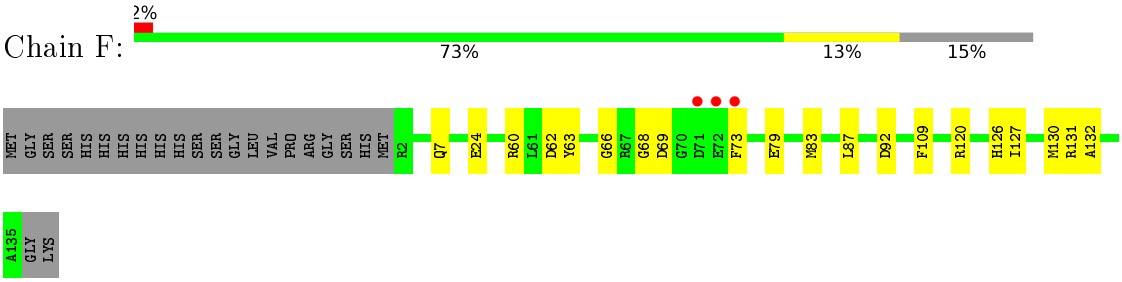


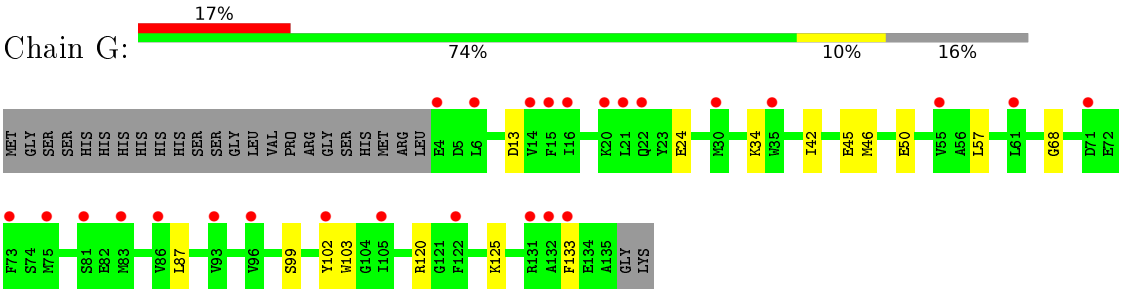
- Molecule 1: Recombination protein uvsY

Chain D:




E134 A135 GLY LYS
• Molecule 1: Recombination protein uvsY
Chain E:
%
73%
13%
14%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS M1 K20 Y23 Y32 W35 L36 N37 K38 M46 K53 G66 R67 G68 D69 F73 S74 L87 D97 W103 G110 L114 M130 F133 E134 A135
GLY LYS


• Molecule 1: Recombination protein uvsY
Chain F:
2%
73%
13%
15%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET R2 Q7 E24 R60 L61 D62 Y63 G66 R67 G68 D69 G70 D71 E72 F73 E79 M83 L87 D92 F109 R120 H126 I127 M130 R131 A132
A135 GLY LYS


• Molecule 1: Recombination protein uvsY
Chain G:
17%
74%
10%
16%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ARG LEU E4 D5 L6 D13 V14 F15 I16 K20 L21 Q22 Y23 E24 M30 K34 M35 I42 E45 M46 E50 V55 A56 L57 L61 G68 D71 E72
F73 S74 M75 S81 E82 M83 V86 L87 V93 V96 S99 Y102 W103 G104 I105 R120 G121 F122 K125 R131 A132 F133 E134 A135 GLY LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	109.26Å 109.22Å 270.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 2.35 46.73 – 2.31	Depositor EDS
% Data completeness (in resolution range)	64.2 (46.73-2.35) 60.8 (46.73-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.83 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.222 , 0.254 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.0	EDS
Estimated twinning fraction	0.500 for -k,-h,-l 0.477 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -k,-h,-l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	10 of 43526 reflections (0.023%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7494	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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 40.97 % 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 2.5299e-04.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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/1100	0.58	0/1473
1	B	0.40	0/1099	0.57	0/1468
1	C	0.44	0/1088	0.62	0/1456
1	D	0.41	0/1100	0.61	1/1470 (0.1%)
1	E	0.37	0/1093	0.58	0/1461
1	F	0.37	0/1084	0.57	0/1452
1	G	0.29	0/1042	0.51	0/1402
All	All	0.38	0/7606	0.58	1/10182 (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	D	61	LEU	CA-CB-CG	5.51	127.98	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1084	0	1073	15	0
1	B	1083	0	1094	20	0
1	C	1072	0	1068	18	0
1	D	1084	0	1091	15	0
1	E	1077	0	1085	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1068	0	1057	14	0
1	G	1026	0	978	11	0
All	All	7494	0	7446	89	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.

The worst 5 of 89 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:TYR:HB2	1:F:69:ASP:HB2	1.74	0.68
1:A:105:ILE:HG12	1:B:43:LYS:HE2	1.75	0.68
1:A:130:MET:HG2	1:B:128:GLN:HG2	1.80	0.64
1:G:42:ILE:HG23	1:G:103:TRP:HE3	1.64	0.63
1:D:128:GLN:OE1	1:D:131:ARG:NH2	2.32	0.62

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	134/157 (85%)	133 (99%)	1 (1%)	0	100	100
1	B	133/157 (85%)	131 (98%)	1 (1%)	1 (1%)	24	26
1	C	132/157 (84%)	130 (98%)	2 (2%)	0	100	100
1	D	133/157 (85%)	131 (98%)	2 (2%)	0	100	100
1	E	133/157 (85%)	131 (98%)	1 (1%)	1 (1%)	24	26
1	F	132/157 (84%)	130 (98%)	2 (2%)	0	100	100
1	G	130/157 (83%)	128 (98%)	1 (1%)	1 (1%)	24	26
All	All	927/1099 (84%)	914 (99%)	10 (1%)	3 (0%)	46	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	68	GLY
1	B	68	GLY
1	E	68	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	113/136 (83%)	112 (99%)	1 (1%)	84	92
1	B	114/136 (84%)	114 (100%)	0	100	100
1	C	113/136 (83%)	112 (99%)	1 (1%)	84	92
1	D	115/136 (85%)	115 (100%)	0	100	100
1	E	113/136 (83%)	113 (100%)	0	100	100
1	F	112/136 (82%)	112 (100%)	0	100	100
1	G	103/136 (76%)	102 (99%)	1 (1%)	82	91
All	All	783/952 (82%)	780 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	C	27	ASN
1	G	50	GLU

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

Mol	Chain	Res	Type
1	B	7	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	136/157 (86%)	0.36	11 (8%)	15	23	27, 42, 64, 79	0
1	B	135/157 (85%)	-0.01	2 (1%)	76	85	19, 30, 64, 68	0
1	C	134/157 (85%)	-0.25	2 (1%)	76	85	14, 23, 42, 82	0
1	D	135/157 (85%)	-0.16	1 (0%)	89	94	12, 28, 46, 64	0
1	E	135/157 (85%)	-0.01	1 (0%)	89	94	19, 33, 56, 79	0
1	F	134/157 (85%)	0.29	3 (2%)	65	77	27, 40, 56, 67	0
1	G	132/157 (84%)	1.20	26 (19%)	1	2	45, 64, 82, 94	0
All	All	941/1099 (85%)	0.20	46 (4%)	33	48	12, 35, 68, 94	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	4	GLU	6.0
1	G	6	LEU	5.0
1	G	133	PHE	4.8
1	E	69	ASP	4.7
1	A	73	PHE	4.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.