wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 03:40 AM EDT

PDB ID	:	4ATW
Title	:	The crystal structure of Arabinofuranosidase
Authors	:	Dumbrepatil, A.; Song, H.-N.; Jung, T.-Y.; Kim, T.-J.; Woo, E.-J.
Deposited on	:	2012-05-10
Resolution	:	3.00 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:

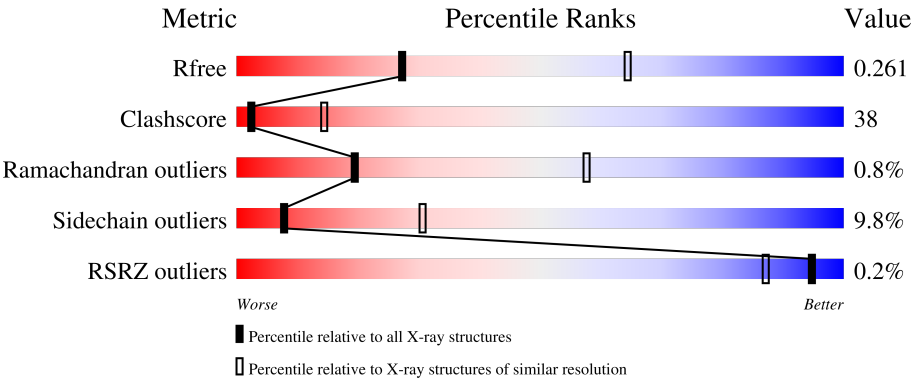
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	482	51% 39% 8%
1	B	482	51% 39% 8%
1	C	482	50% 40% 9%
1	D	482	50% 39% 9%
1	E	482	% 50% 42% 7%

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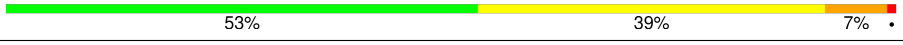
Mol	Chain	Length	Quality of chain
1	F	482	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23256 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 ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	B	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	C	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	D	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	E	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			
1	F	481	Total	C	N	O	S	0	0	0
			3876	2486	646	729	15			

There are 6 discrepancies between the modelled and reference sequences:

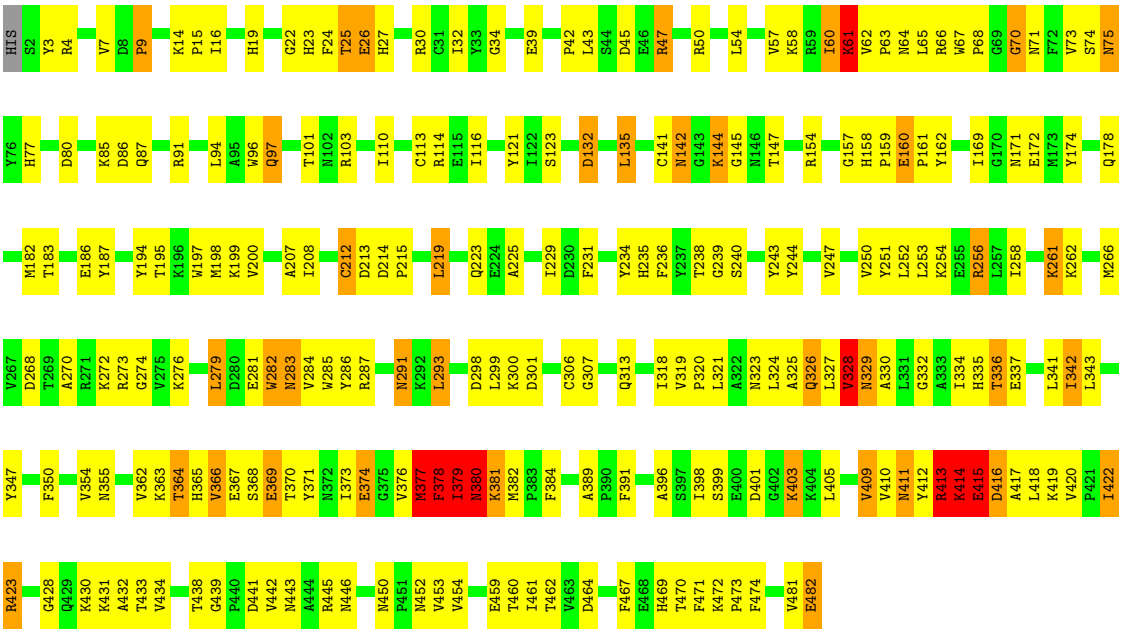
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP G4FHJ5
B	1	HIS	-	expression tag	UNP G4FHJ5
C	1	HIS	-	expression tag	UNP G4FHJ5
D	1	HIS	-	expression tag	UNP G4FHJ5
E	1	HIS	-	expression tag	UNP G4FHJ5
F	1	HIS	-	expression tag	UNP G4FHJ5

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.

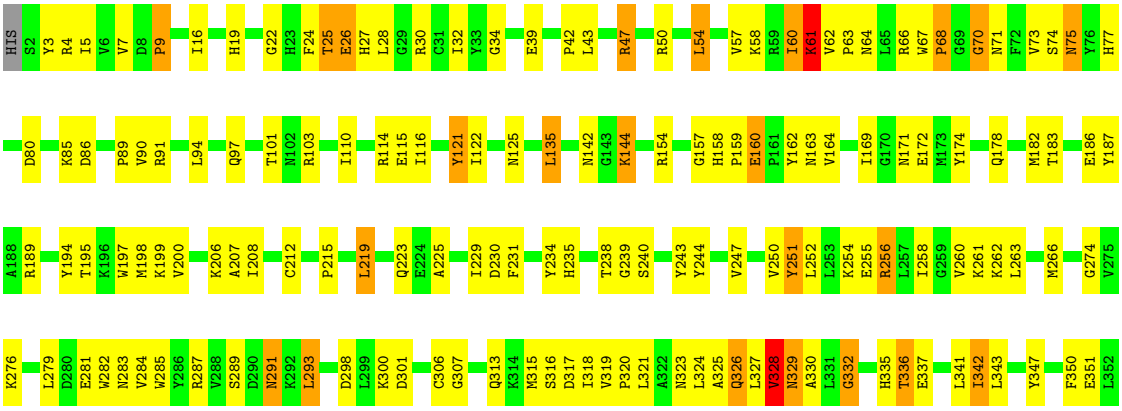
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

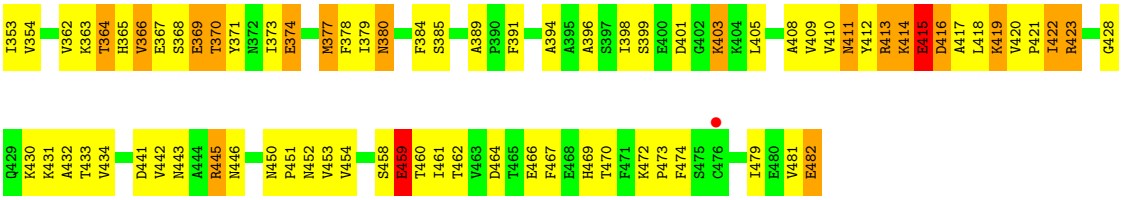
Chain A:



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

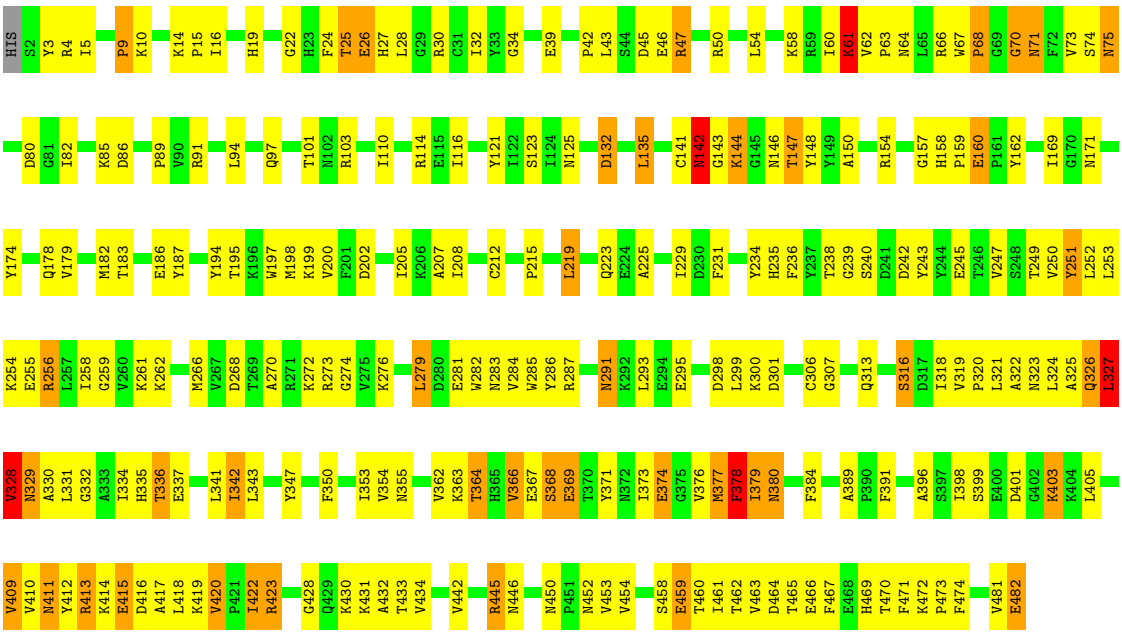
Chain B:





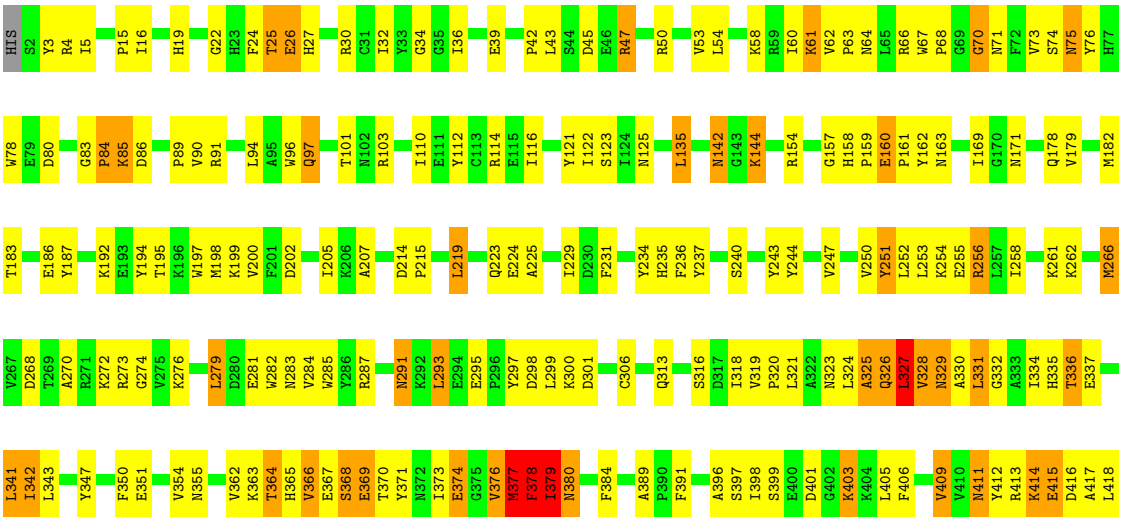
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

Chain C:



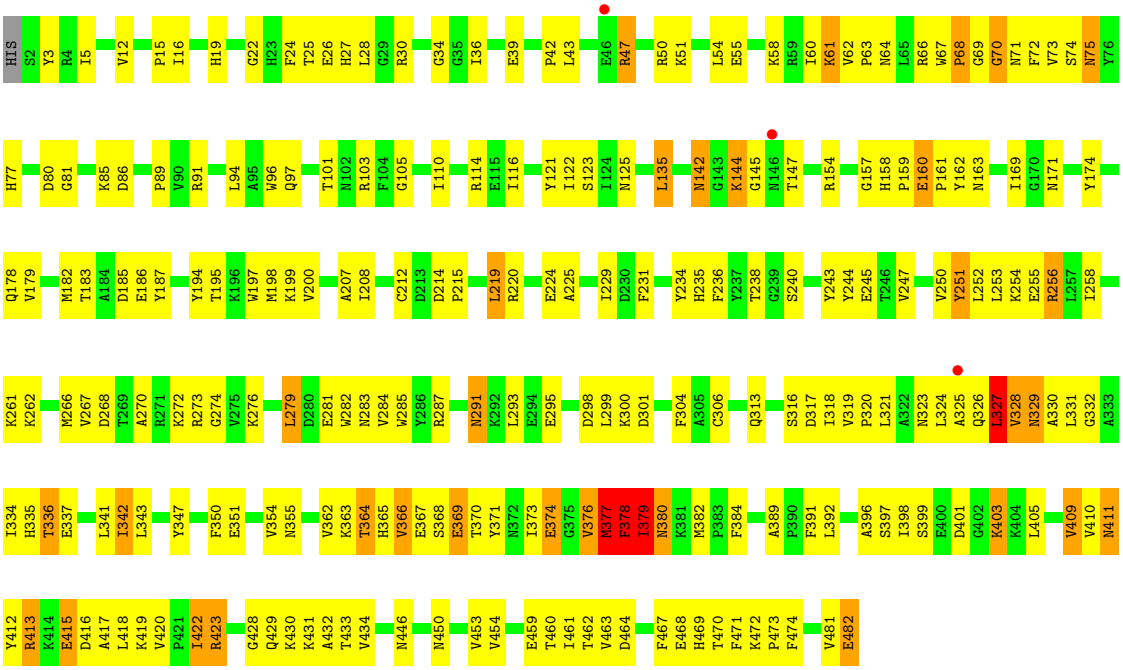
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

Chain D:



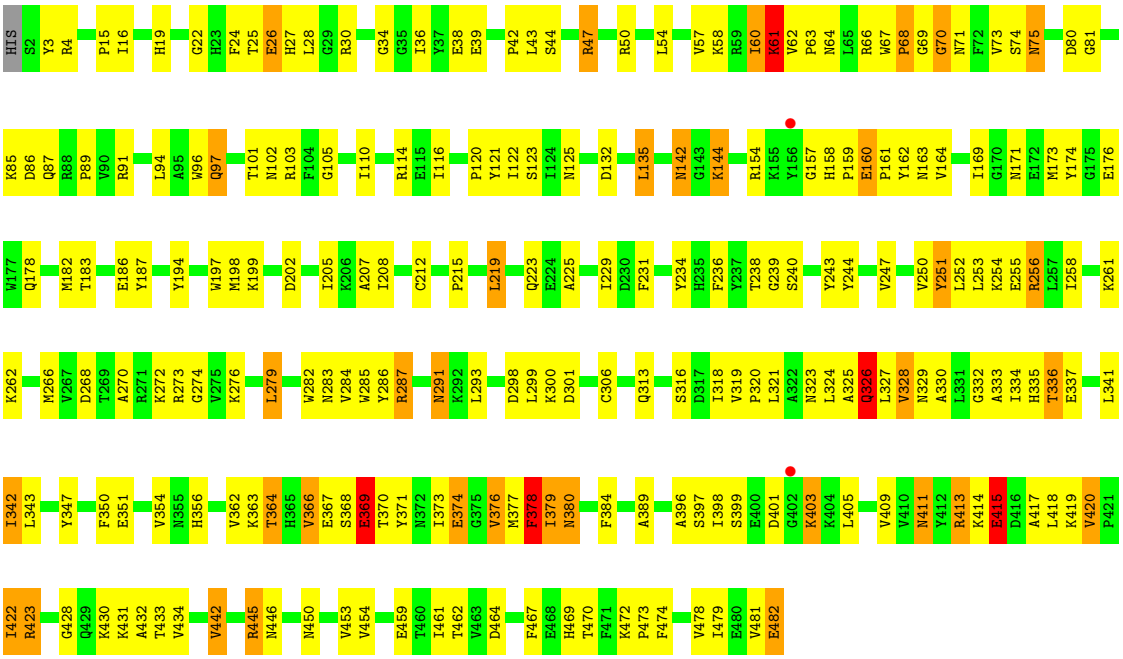
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

Chain E:



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

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	103.71Å 161.54Å 112.60Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	29.94 – 3.00 29.94 – 2.99	Depositor EDS
% Data completeness (in resolution range)	84.5 (29.94-3.00) 84.2 (29.94-2.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.262 0.227 , 0.261	Depositor DCC
R_{free} test set	4430 reflections (6.60%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.9	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	0.87	EDS
Total number of atoms	23256	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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

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	1.04	21/3971 (0.5%)	1.01	31/5383 (0.6%)
1	B	0.73	5/3971 (0.1%)	0.98	22/5383 (0.4%)
1	C	0.99	24/3971 (0.6%)	0.96	24/5383 (0.4%)
1	D	1.10	37/3971 (0.9%)	1.04	31/5383 (0.6%)
1	E	0.84	16/3971 (0.4%)	0.95	17/5383 (0.3%)
1	F	0.81	11/3971 (0.3%)	0.91	16/5383 (0.3%)
All	All	0.93	114/23826 (0.5%)	0.97	141/32298 (0.4%)

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	1	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	3
All	All	1	9

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	VAL	CB-CG1	-19.15	1.12	1.52
1	A	328	VAL	CA-CB	-18.55	1.15	1.54
1	D	26	GLU	C-N	-17.58	0.93	1.34
1	A	378	PHE	CE2-CZ	-16.47	1.06	1.37
1	D	328	VAL	CB-CG2	-16.30	1.18	1.52

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	ASN	N-CA-C	15.22	152.09	111.00
1	D	25	THR	O-C-N	-13.37	101.31	122.70
1	A	379	ILE	CB-CA-C	-12.96	85.69	111.60
1	D	325	ALA	CB-CA-C	12.94	129.50	110.10
1	E	376	VAL	CB-CA-C	-12.41	87.82	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	377	MET	CA

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	MET	Mainchain
1	B	251	TYR	Sidechain
1	C	251	TYR	Sidechain
1	D	251	TYR	Sidechain
1	D	327	LEU	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	3876	0	3788	292	0
1	B	3876	0	3788	290	0
1	C	3876	0	3788	276	2
1	D	3876	0	3787	308	0
1	E	3876	0	3789	300	2
1	F	3876	0	3788	302	0
All	All	23256	0	22728	1727	2

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 38.

The worst 5 of 1727 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:24:PHE:CD2	1:E:325:ALA:HB1	1.34	1.62
1:E:419:LYS:CG	1:E:470:THR:CG2	1.80	1.58
1:B:410:VAL:HG11	1:B:412:TYR:CZ	1.23	1.57
1:F:419:LYS:CG	1:F:470:THR:CG2	1.77	1.57
1:E:24:PHE:HD2	1:E:325:ALA:CB	1.17	1.57

All (2) 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:C:144:LYS:CE	1:E:431:LYS:CE[1_556]	1.60	0.60
1:C:144:LYS:CE	1:E:431:LYS:NZ[1_556]	1.90	0.30

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	476/482 (99%)	409 (86%)	62 (13%)	5 (1%)	14	50
1	B	476/482 (99%)	409 (86%)	61 (13%)	6 (1%)	12	45
1	C	476/482 (99%)	410 (86%)	61 (13%)	5 (1%)	14	50
1	D	476/482 (99%)	403 (85%)	70 (15%)	3 (1%)	25	64
1	E	476/482 (99%)	407 (86%)	66 (14%)	3 (1%)	25	64
1	F	476/482 (99%)	406 (85%)	68 (14%)	2 (0%)	34	72
All	All	2856/2892 (99%)	2444 (86%)	388 (14%)	24 (1%)	19	57

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	VAL
1	A	379	ILE
1	B	172	GLU

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Mol	Chain	Res	Type
1	C	465	THR
1	E	328	VAL

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	417/418 (100%)	376 (90%)	41 (10%)	8	30
1	B	417/418 (100%)	375 (90%)	42 (10%)	7	29
1	C	417/418 (100%)	374 (90%)	43 (10%)	7	28
1	D	417/418 (100%)	376 (90%)	41 (10%)	8	30
1	E	417/418 (100%)	378 (91%)	39 (9%)	8	32
1	F	417/418 (100%)	377 (90%)	40 (10%)	8	32
All	All	2502/2508 (100%)	2256 (90%)	246 (10%)	8	30

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	409	VAL
1	F	291	ASN
1	D	321	LEU
1	F	261	LYS
1	F	413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	326	GLN
1	F	380	ASN
1	E	388	ASN
1	F	77	HIS
1	F	446	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	A	3
1	B	3
1	D	3
1	F	2
1	E	2

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	157:GLY	C	158:HIS	N	3.85
1	F	157:GLY	C	158:HIS	N	3.82
1	A	157:GLY	C	158:HIS	N	3.80
1	B	157:GLY	C	158:HIS	N	3.80
1	E	157:GLY	C	158:HIS	N	3.79

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	481/482 (99%)	-0.71	0 100 100	14, 42, 75, 115	0
1	B	481/482 (99%)	-0.55	1 (0%) 95 87	15, 47, 92, 117	0
1	C	481/482 (99%)	-0.69	0 100 100	17, 40, 66, 88	0
1	D	481/482 (99%)	-0.59	0 100 100	17, 54, 85, 110	0
1	E	481/482 (99%)	-0.33	3 (0%) 89 72	31, 67, 93, 115	0
1	F	481/482 (99%)	-0.33	2 (0%) 92 79	33, 64, 91, 129	0
All	All	2886/2892 (99%)	-0.53	6 (0%) 95 87	14, 52, 88, 129	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	146	ASN	3.2
1	F	402	GLY	3.1
1	E	325	ALA	2.3
1	F	156	TYR	2.2
1	B	476	CYS	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.