Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2017 – 07:45 PM EST

PDB ID	:	5HY4
Title	:	Structure-function analysis of functionally diverse members of the cyclic amide hydrolase family of Toblerone fold enzymes
Authors	:	Peat, T.S.; Balotra, S.; Wilding, M.; Newman, J.; Scott, C.
Deposited on	:	2016-02-01
Resolution	:	2.56 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
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:

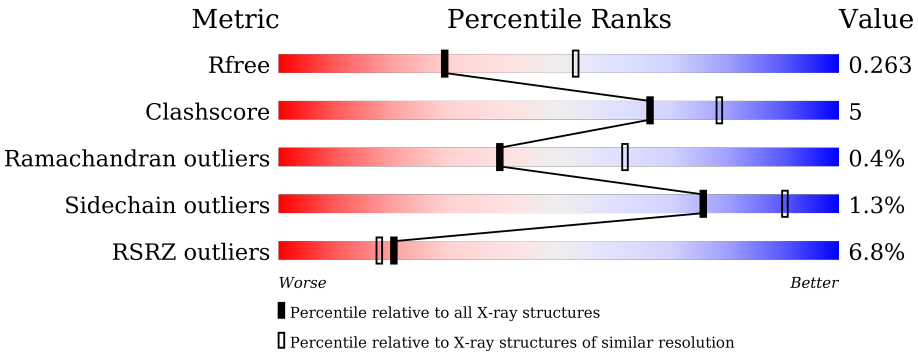
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.56 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	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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	410	5% 80% 8% 12%
1	B	410	3% 80% 6% • 12%
1	C	410	5% 74% 9% • 15%
1	D	410	5% 74% 7% • 19%
1	E	410	3% 80% 5% 15%
1	F	410	7% 73% 11% • 15%

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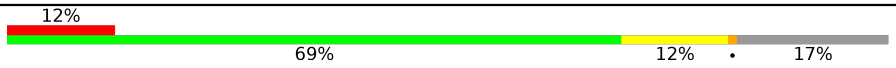
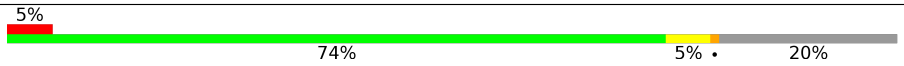
Mol	Chain	Length	Quality of chain
1	G	410	
1	H	410	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19841 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 Ring-opening amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	1	0
			2565	1590	463	501	11			
1	B	360	Total	C	N	O	S	0	2	0
			2586	1606	472	497	11			
1	C	348	Total	C	N	O	S	0	2	0
			2430	1509	437	473	11			
1	D	333	Total	C	N	O	S	0	2	0
			2349	1457	423	459	10			
1	E	349	Total	C	N	O	S	0	3	0
			2482	1538	451	483	10			
1	F	350	Total	C	N	O	S	0	1	0
			2461	1529	439	482	11			
1	G	340	Total	C	N	O	S	0	1	0
			2371	1472	421	467	11			
1	H	328	Total	C	N	O	S	0	2	0
			2341	1454	424	452	11			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E3JD18
A	-18	GLY	-	expression tag	UNP E3JD18
A	-17	SER	-	expression tag	UNP E3JD18
A	-16	SER	-	expression tag	UNP E3JD18
A	-15	HIS	-	expression tag	UNP E3JD18
A	-14	HIS	-	expression tag	UNP E3JD18
A	-13	HIS	-	expression tag	UNP E3JD18
A	-12	HIS	-	expression tag	UNP E3JD18
A	-11	HIS	-	expression tag	UNP E3JD18
A	-10	HIS	-	expression tag	UNP E3JD18
A	-9	SER	-	expression tag	UNP E3JD18
A	-8	SER	-	expression tag	UNP E3JD18
A	-7	GLY	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP E3JD18
A	-5	VAL	-	expression tag	UNP E3JD18
A	-4	PRO	-	expression tag	UNP E3JD18
A	-3	ARG	-	expression tag	UNP E3JD18
A	-2	GLY	-	expression tag	UNP E3JD18
A	-1	SER	-	expression tag	UNP E3JD18
A	0	HIS	-	expression tag	UNP E3JD18
B	-19	MET	-	initiating methionine	UNP E3JD18
B	-18	GLY	-	expression tag	UNP E3JD18
B	-17	SER	-	expression tag	UNP E3JD18
B	-16	SER	-	expression tag	UNP E3JD18
B	-15	HIS	-	expression tag	UNP E3JD18
B	-14	HIS	-	expression tag	UNP E3JD18
B	-13	HIS	-	expression tag	UNP E3JD18
B	-12	HIS	-	expression tag	UNP E3JD18
B	-11	HIS	-	expression tag	UNP E3JD18
B	-10	HIS	-	expression tag	UNP E3JD18
B	-9	SER	-	expression tag	UNP E3JD18
B	-8	SER	-	expression tag	UNP E3JD18
B	-7	GLY	-	expression tag	UNP E3JD18
B	-6	LEU	-	expression tag	UNP E3JD18
B	-5	VAL	-	expression tag	UNP E3JD18
B	-4	PRO	-	expression tag	UNP E3JD18
B	-3	ARG	-	expression tag	UNP E3JD18
B	-2	GLY	-	expression tag	UNP E3JD18
B	-1	SER	-	expression tag	UNP E3JD18
B	0	HIS	-	expression tag	UNP E3JD18
C	-19	MET	-	initiating methionine	UNP E3JD18
C	-18	GLY	-	expression tag	UNP E3JD18
C	-17	SER	-	expression tag	UNP E3JD18
C	-16	SER	-	expression tag	UNP E3JD18
C	-15	HIS	-	expression tag	UNP E3JD18
C	-14	HIS	-	expression tag	UNP E3JD18
C	-13	HIS	-	expression tag	UNP E3JD18
C	-12	HIS	-	expression tag	UNP E3JD18
C	-11	HIS	-	expression tag	UNP E3JD18
C	-10	HIS	-	expression tag	UNP E3JD18
C	-9	SER	-	expression tag	UNP E3JD18
C	-8	SER	-	expression tag	UNP E3JD18
C	-7	GLY	-	expression tag	UNP E3JD18
C	-6	LEU	-	expression tag	UNP E3JD18
C	-5	VAL	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP E3JD18
C	-3	ARG	-	expression tag	UNP E3JD18
C	-2	GLY	-	expression tag	UNP E3JD18
C	-1	SER	-	expression tag	UNP E3JD18
C	0	HIS	-	expression tag	UNP E3JD18
D	-19	MET	-	initiating methionine	UNP E3JD18
D	-18	GLY	-	expression tag	UNP E3JD18
D	-17	SER	-	expression tag	UNP E3JD18
D	-16	SER	-	expression tag	UNP E3JD18
D	-15	HIS	-	expression tag	UNP E3JD18
D	-14	HIS	-	expression tag	UNP E3JD18
D	-13	HIS	-	expression tag	UNP E3JD18
D	-12	HIS	-	expression tag	UNP E3JD18
D	-11	HIS	-	expression tag	UNP E3JD18
D	-10	HIS	-	expression tag	UNP E3JD18
D	-9	SER	-	expression tag	UNP E3JD18
D	-8	SER	-	expression tag	UNP E3JD18
D	-7	GLY	-	expression tag	UNP E3JD18
D	-6	LEU	-	expression tag	UNP E3JD18
D	-5	VAL	-	expression tag	UNP E3JD18
D	-4	PRO	-	expression tag	UNP E3JD18
D	-3	ARG	-	expression tag	UNP E3JD18
D	-2	GLY	-	expression tag	UNP E3JD18
D	-1	SER	-	expression tag	UNP E3JD18
D	0	HIS	-	expression tag	UNP E3JD18
E	-19	MET	-	initiating methionine	UNP E3JD18
E	-18	GLY	-	expression tag	UNP E3JD18
E	-17	SER	-	expression tag	UNP E3JD18
E	-16	SER	-	expression tag	UNP E3JD18
E	-15	HIS	-	expression tag	UNP E3JD18
E	-14	HIS	-	expression tag	UNP E3JD18
E	-13	HIS	-	expression tag	UNP E3JD18
E	-12	HIS	-	expression tag	UNP E3JD18
E	-11	HIS	-	expression tag	UNP E3JD18
E	-10	HIS	-	expression tag	UNP E3JD18
E	-9	SER	-	expression tag	UNP E3JD18
E	-8	SER	-	expression tag	UNP E3JD18
E	-7	GLY	-	expression tag	UNP E3JD18
E	-6	LEU	-	expression tag	UNP E3JD18
E	-5	VAL	-	expression tag	UNP E3JD18
E	-4	PRO	-	expression tag	UNP E3JD18
E	-3	ARG	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E3JD18
E	-1	SER	-	expression tag	UNP E3JD18
E	0	HIS	-	expression tag	UNP E3JD18
F	-19	MET	-	initiating methionine	UNP E3JD18
F	-18	GLY	-	expression tag	UNP E3JD18
F	-17	SER	-	expression tag	UNP E3JD18
F	-16	SER	-	expression tag	UNP E3JD18
F	-15	HIS	-	expression tag	UNP E3JD18
F	-14	HIS	-	expression tag	UNP E3JD18
F	-13	HIS	-	expression tag	UNP E3JD18
F	-12	HIS	-	expression tag	UNP E3JD18
F	-11	HIS	-	expression tag	UNP E3JD18
F	-10	HIS	-	expression tag	UNP E3JD18
F	-9	SER	-	expression tag	UNP E3JD18
F	-8	SER	-	expression tag	UNP E3JD18
F	-7	GLY	-	expression tag	UNP E3JD18
F	-6	LEU	-	expression tag	UNP E3JD18
F	-5	VAL	-	expression tag	UNP E3JD18
F	-4	PRO	-	expression tag	UNP E3JD18
F	-3	ARG	-	expression tag	UNP E3JD18
F	-2	GLY	-	expression tag	UNP E3JD18
F	-1	SER	-	expression tag	UNP E3JD18
F	0	HIS	-	expression tag	UNP E3JD18
G	-19	MET	-	initiating methionine	UNP E3JD18
G	-18	GLY	-	expression tag	UNP E3JD18
G	-17	SER	-	expression tag	UNP E3JD18
G	-16	SER	-	expression tag	UNP E3JD18
G	-15	HIS	-	expression tag	UNP E3JD18
G	-14	HIS	-	expression tag	UNP E3JD18
G	-13	HIS	-	expression tag	UNP E3JD18
G	-12	HIS	-	expression tag	UNP E3JD18
G	-11	HIS	-	expression tag	UNP E3JD18
G	-10	HIS	-	expression tag	UNP E3JD18
G	-9	SER	-	expression tag	UNP E3JD18
G	-8	SER	-	expression tag	UNP E3JD18
G	-7	GLY	-	expression tag	UNP E3JD18
G	-6	LEU	-	expression tag	UNP E3JD18
G	-5	VAL	-	expression tag	UNP E3JD18
G	-4	PRO	-	expression tag	UNP E3JD18
G	-3	ARG	-	expression tag	UNP E3JD18
G	-2	GLY	-	expression tag	UNP E3JD18
G	-1	SER	-	expression tag	UNP E3JD18

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP E3JD18
H	-19	MET	-	initiating methionine	UNP E3JD18
H	-18	GLY	-	expression tag	UNP E3JD18
H	-17	SER	-	expression tag	UNP E3JD18
H	-16	SER	-	expression tag	UNP E3JD18
H	-15	HIS	-	expression tag	UNP E3JD18
H	-14	HIS	-	expression tag	UNP E3JD18
H	-13	HIS	-	expression tag	UNP E3JD18
H	-12	HIS	-	expression tag	UNP E3JD18
H	-11	HIS	-	expression tag	UNP E3JD18
H	-10	HIS	-	expression tag	UNP E3JD18
H	-9	SER	-	expression tag	UNP E3JD18
H	-8	SER	-	expression tag	UNP E3JD18
H	-7	GLY	-	expression tag	UNP E3JD18
H	-6	LEU	-	expression tag	UNP E3JD18
H	-5	VAL	-	expression tag	UNP E3JD18
H	-4	PRO	-	expression tag	UNP E3JD18
H	-3	ARG	-	expression tag	UNP E3JD18
H	-2	GLY	-	expression tag	UNP E3JD18
H	-1	SER	-	expression tag	UNP E3JD18
H	0	HIS	-	expression tag	UNP E3JD18

- Molecule 2 is water.

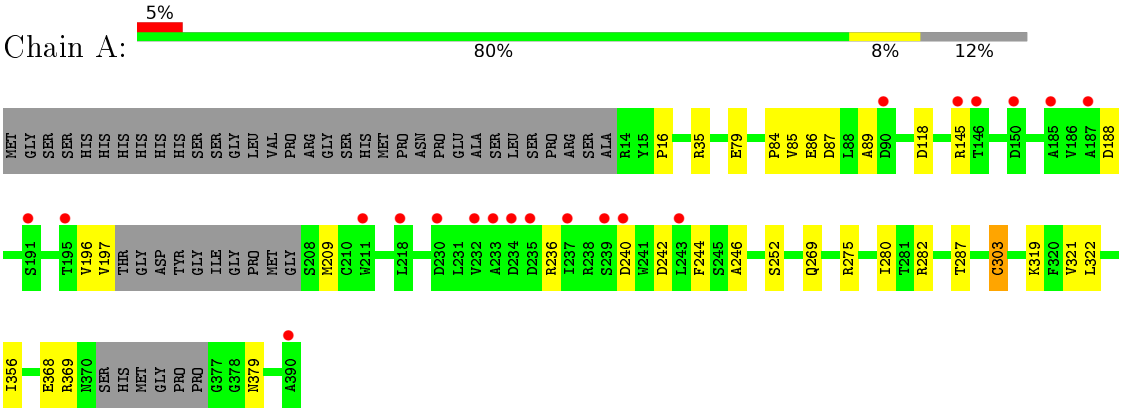
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	50	Total O 50 50	0	0
2	B	27	Total O 27 27	0	0
2	C	25	Total O 25 25	0	0
2	D	21	Total O 21 21	0	0
2	E	53	Total O 53 53	0	0
2	F	37	Total O 37 37	0	0
2	G	11	Total O 11 11	0	0
2	H	32	Total O 32 32	0	0

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.

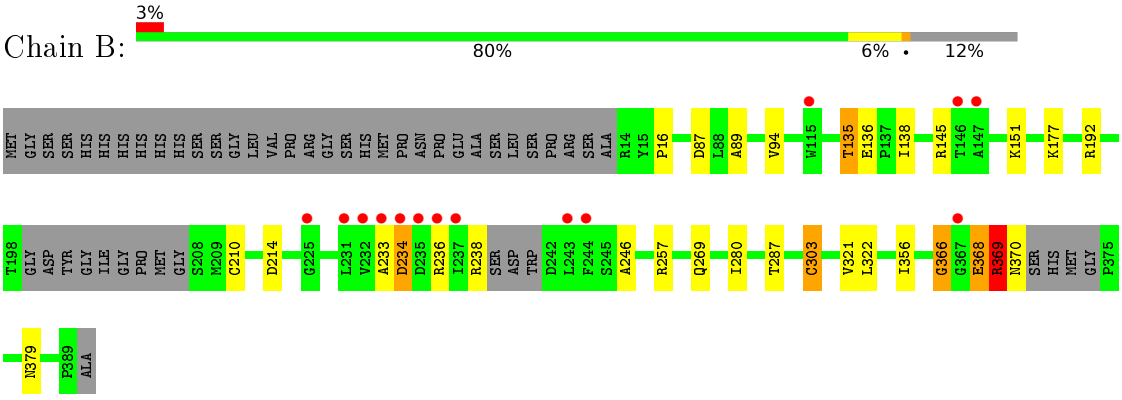
- Molecule 1: Ring-opening amidohydrolase

Chain A:



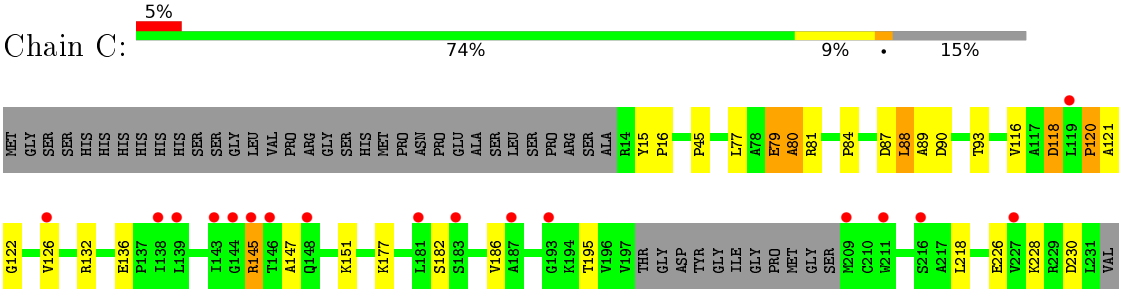
- Molecule 1: Ring-opening amidohydrolase

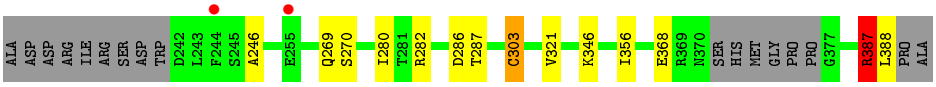
Chain B:



- Molecule 1: Ring-opening amidohydrolase

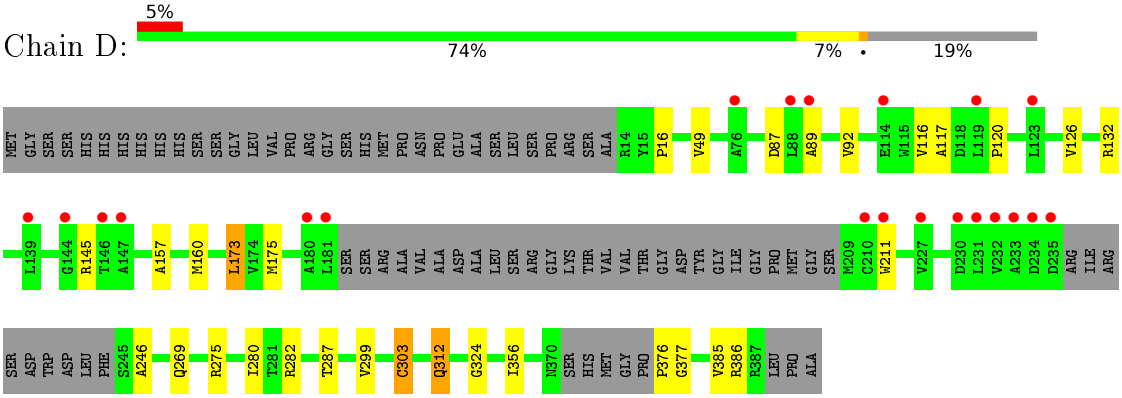
Chain C:





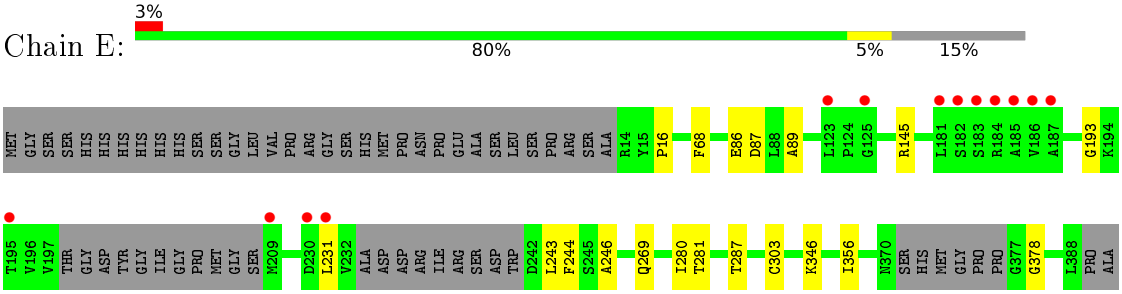
• Molecule 1: Ring-opening amidohydrolase

Chain D:



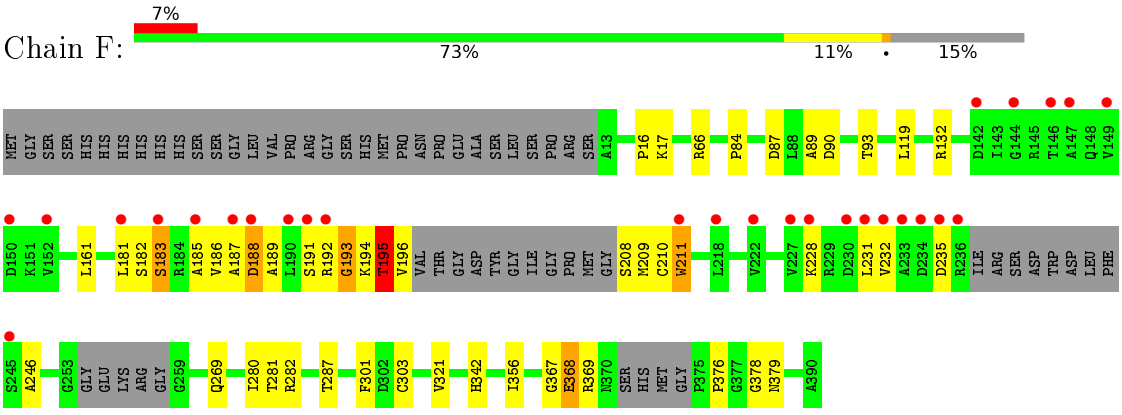
• Molecule 1: Ring-opening amidohydrolase

Chain E:



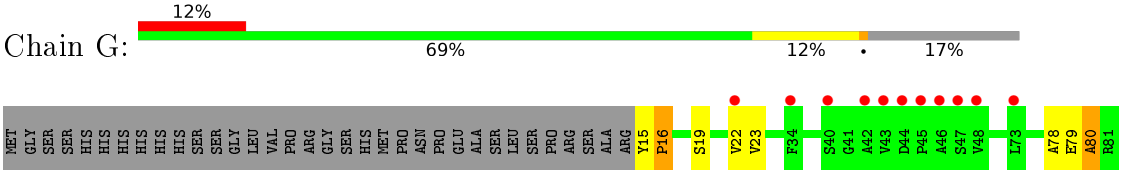
• Molecule 1: Ring-opening amidohydrolase

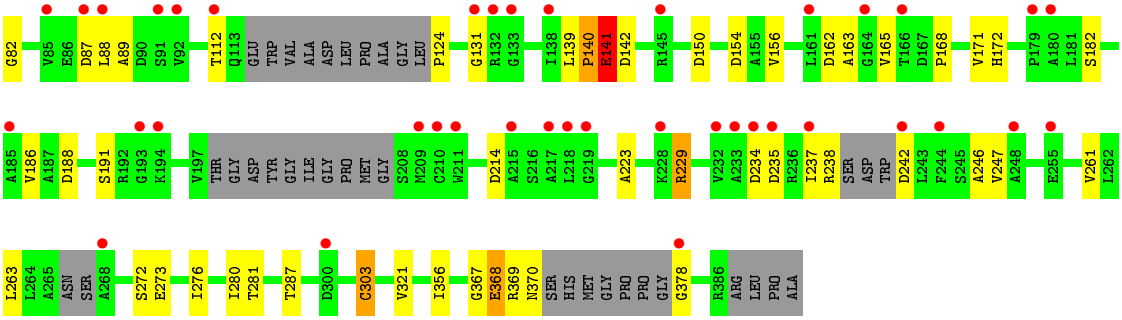
Chain F:



• Molecule 1: Ring-opening amidohydrolase

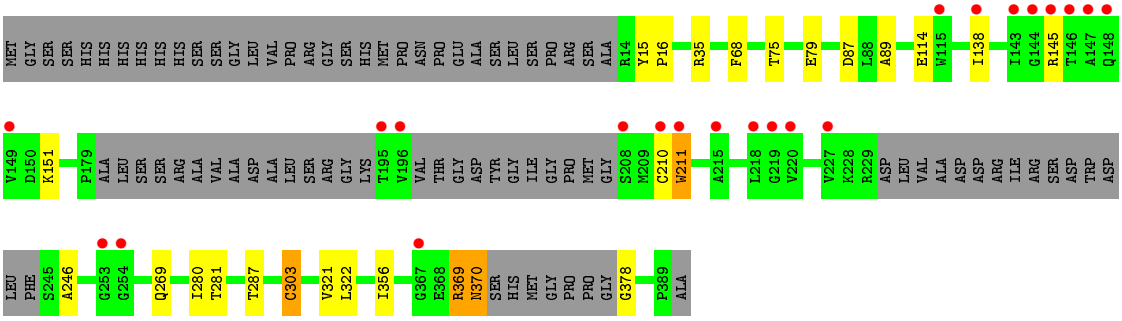
Chain G:





- Molecule 1: Ring-opening amidohydrolase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.76Å 105.80Å 299.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 2.56 45.95 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.70-2.56) 99.4 (45.95-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.229 , 0.263 0.232 , 0.263	Depositor DCC
R_{free} test set	4666 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19841	wwPDB-VP
Average B, all atoms (Å^2)	55.0	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 22.83 % 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 5.2675e-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

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	0.65	0/2604	0.83	6/3550 (0.2%)
1	B	0.67	0/2627	0.83	6/3578 (0.2%)
1	C	0.68	1/2466 (0.0%)	0.85	7/3366 (0.2%)
1	D	0.63	0/2385	0.81	4/3254 (0.1%)
1	E	0.64	0/2517	0.82	2/3429 (0.1%)
1	F	0.68	0/2500	0.80	2/3413 (0.1%)
1	G	0.70	0/2402	0.86	4/3273 (0.1%)
1	H	0.66	1/2377 (0.0%)	0.79	1/3239 (0.0%)
All	All	0.66	2/19878 (0.0%)	0.82	32/27102 (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	B	0	2
1	C	0	8
1	D	0	4
1	F	0	4
1	G	0	4
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	211	TRP	CB-CG	-5.59	1.40	1.50
1	C	226	GLU	CD-OE1	-5.34	1.19	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	145	ARG	NE-CZ-NH1	9.01	124.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	145	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	G	235	ASP	CB-CG-OD1	8.14	125.63	118.30
1	G	154	ASP	CB-CG-OD2	7.80	125.32	118.30
1	G	79	GLU	CB-CA-C	7.65	125.70	110.40
1	G	235	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	C	218	LEU	CB-CG-CD2	-7.33	98.54	111.00
1	A	188	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	188	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	C	218	LEU	CB-CG-CD1	7.04	122.98	111.00
1	B	234	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	145	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	D	173	LEU	CB-CG-CD1	6.64	122.29	111.00
1	B	145	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	C	79	GLU	CB-CA-C	-6.11	98.18	110.40
1	F	161	LEU	CB-CG-CD1	6.08	121.33	111.00
1	A	145	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	C	387	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	F	209	MET	CG-SD-CE	5.83	109.53	100.20
1	A	282	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	282	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	257	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	135	THR	CA-CB-CG2	-5.46	104.76	112.40
1	H	145	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	387	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	D	312	GLN	CB-CA-C	5.24	120.88	110.40
1	A	118	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	145	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	218	LEU	CA-CB-CG	5.12	127.07	115.30
1	C	145	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	D	145	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	366	GLY	CA-C-N	5.02	126.23	116.20

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	366	GLY	Peptide
1	B	369	ARG	Peptide
1	C	118	ASP	Peptide
1	C	120	PRO	Peptide
1	C	121	ALA	Peptide
1	C	122	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	387	ARG	Peptide
1	C	79	GLU	Peptide
1	C	80	ALA	Mainchain
1	C	88	LEU	Peptide
1	D	116	VAL	Peptide
1	D	117	ALA	Peptide
1	D	120	PRO	Peptide
1	D	377	GLY	Peptide
1	F	193	GLY	Peptide
1	F	195	THR	Peptide
1	F	368	GLU	Peptide
1	F	369	ARG	Peptide
1	G	124	PRO	Peptide
1	G	140	PRO	Peptide
1	G	242	ASP	Peptide
1	G	80	ALA	Peptide

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	2565	0	2528	16	0
1	B	2586	0	2575	22	1
1	C	2430	0	2359	27	0
1	D	2349	0	2306	17	0
1	E	2482	0	2451	10	1
1	F	2461	0	2414	39	0
1	G	2371	0	2318	43	0
1	H	2341	0	2317	20	0
2	A	50	0	0	1	0
2	B	27	0	0	0	0
2	C	25	0	0	1	0
2	D	21	0	0	0	0
2	E	53	0	0	1	0
2	F	37	0	0	2	0
2	G	11	0	0	0	0
2	H	32	0	0	0	0
All	All	19841	0	19268	189	1

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 5.

All (189) 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:H:35[B]:ARG:NH2	1:H:79[B]:GLU:OE1	1.62	1.31
1:G:172:HIS:O	1:G:247:VAL:HG13	1.43	1.15
1:G:150:ASP:OD1	1:G:229:ARG:NH1	1.82	1.12
1:C:87:ASP:O	1:C:89:ALA:N	1.97	0.97
1:H:35[B]:ARG:HH21	1:H:79[B]:GLU:CD	1.73	0.91
1:C:90:ASP:O	1:C:132:ARG:NH2	2.05	0.89
1:H:35[B]:ARG:NH2	1:H:79[B]:GLU:CD	2.28	0.84
1:B:322:LEU:HD12	1:B:369:ARG:HD2	1.59	0.84
1:C:87:ASP:C	1:C:89:ALA:H	1.80	0.81
1:D:173:LEU:HD21	1:D:175:MET:HG3	1.67	0.77
1:F:183:SER:O	1:F:186:VAL:HG12	1.86	0.76
1:H:321:VAL:HG11	1:H:370:ASN:HB2	1.67	0.75
1:G:168:PRO:O	1:G:171:VAL:HG12	1.87	0.75
1:C:87:ASP:C	1:C:89:ALA:N	2.39	0.74
1:G:172:HIS:C	1:G:247:VAL:HG13	2.07	0.74
1:F:93:THR:OG1	1:F:132:ARG:NH1	2.21	0.74
1:F:193:GLY:HA2	1:F:194:LYS:CB	2.18	0.74
1:B:214:ASP:OD2	1:B:238:ARG:NH1	2.20	0.73
1:G:19:SER:OG	1:G:112:THR:OG1	2.06	0.73
1:G:172:HIS:CD2	1:G:276:ILE:HG23	2.24	0.72
1:F:181:LEU:HB2	1:F:208:SER:HB2	1.73	0.71
1:C:93:THR:OG1	1:C:132:ARG:NH1	2.23	0.70
1:G:156:VAL:HG23	1:G:223:ALA:CB	2.23	0.69
1:F:188:ASP:O	1:F:192:ARG:HG3	1.93	0.68
1:G:156:VAL:CG2	1:G:223:ALA:CB	2.72	0.67
1:C:136:GLU:HB2	1:C:151:LYS:HD3	1.77	0.67
1:B:94:VAL:O	1:B:177:LYS:NZ	2.28	0.66
1:C:388:LEU:O	1:C:388:LEU:HD23	1.97	0.65
1:A:319:LYS:NZ	1:A:368:GLU:OE2	2.23	0.64
1:A:236:ARG:NH2	1:A:240:ASP:OD2	2.29	0.64
1:G:150:ASP:CG	1:G:229:ARG:HH12	2.01	0.64
1:H:322:LEU:HD12	1:H:369:ARG:HG3	1.77	0.64
1:C:182:SER:O	1:C:186:VAL:HG23	1.98	0.64
1:G:156:VAL:HG21	1:G:223:ALA:HB3	1.78	0.64
1:C:282:ARG:HD3	1:C:286:ASP:OD2	1.99	0.62
1:C:321:VAL:HG22	1:C:368:GLU:HG2	1.82	0.62
1:F:192:ARG:NH1	2:F:401:HOH:O	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:ALA:O	1:F:194:LYS:CB	2.49	0.61
1:F:84:PRO:HD2	1:F:87:ASP:OD2	2.01	0.61
1:B:368:GLU:C	1:B:369:ARG:HD3	2.22	0.60
1:F:189:ALA:O	1:F:193:GLY:N	2.34	0.60
1:G:229:ARG:O	1:G:229:ARG:HD2	2.02	0.60
1:G:171:VAL:HG23	1:G:263:LEU:HD21	1.84	0.60
1:A:322:LEU:HD12	1:A:369:ARG:HG2	1.83	0.59
1:A:84:PRO:HD2	1:A:87:ASP:OD2	2.01	0.59
1:B:369:ARG:HB2	1:B:369:ARG:HH11	1.68	0.59
1:G:156:VAL:CG2	1:G:223:ALA:HB3	2.32	0.58
1:G:172:HIS:O	1:G:247:VAL:CG1	2.36	0.58
1:C:145:ARG:NH2	1:C:195:THR:O	2.37	0.57
1:A:303:CYS:HB3	1:C:303:CYS:SG	2.45	0.56
1:G:214:ASP:OD2	1:G:238:ARG:HG2	2.04	0.56
1:H:210:CYS:SG	1:H:211:TRP:CD1	2.98	0.56
1:C:387:ARG:N	1:C:388:LEU:HA	2.20	0.56
1:G:139:LEU:HB3	1:G:141:GLU:HG3	1.87	0.56
1:A:287:THR:HB	1:A:356:ILE:HD11	1.87	0.56
1:B:322:LEU:O	1:B:370:ASN:HB2	2.06	0.56
1:F:182:SER:O	1:F:185:ALA:HB3	2.06	0.56
1:A:35[B]:ARG:NH2	1:A:79:GLU:OE2	2.38	0.55
1:G:172:HIS:C	1:G:247:VAL:CG1	2.73	0.55
1:G:287:THR:HB	1:G:356:ILE:HD11	1.89	0.55
1:F:193:GLY:CA	1:F:194:LYS:CB	2.85	0.55
1:C:287:THR:HB	1:C:356:ILE:HD11	1.89	0.55
1:G:22:VAL:C	1:G:23:VAL:HG23	2.26	0.55
1:D:287:THR:HB	1:D:356:ILE:HD11	1.89	0.54
1:G:246:ALA:HB1	1:G:280:ILE:HD11	1.89	0.54
1:D:312:GLN:O	1:D:385:VAL:HG13	2.08	0.54
1:B:287:THR:HB	1:B:356:ILE:HD11	1.89	0.54
1:F:287:THR:HB	1:F:356:ILE:HD11	1.89	0.54
1:B:87:ASP:C	1:B:89:ALA:H	2.11	0.54
1:H:287:THR:HB	1:H:356:ILE:HD11	1.89	0.54
1:G:87:ASP:C	1:G:89:ALA:H	2.12	0.53
1:F:228:LYS:HB2	1:F:231:LEU:HD13	1.90	0.53
1:G:321:VAL:HG13	1:G:369:ARG:HA	1.90	0.53
1:C:246:ALA:HB1	1:C:280:ILE:HD11	1.91	0.53
1:E:287:THR:HB	1:E:356:ILE:HD11	1.89	0.53
1:C:77:LEU:O	1:C:81:ARG:HG3	2.09	0.53
1:B:321:VAL:HG22	1:B:379:ASN:OD1	2.09	0.52
1:D:87:ASP:C	1:D:89:ALA:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:ALA:HB1	1:E:280:ILE:HD11	1.91	0.52
1:G:87:ASP:O	1:G:89:ALA:N	2.42	0.52
1:F:182:SER:HB2	1:F:185:ALA:HB2	1.92	0.52
1:G:188:ASP:O	1:G:191:SER:HB3	2.10	0.51
1:F:194:LYS:O	1:F:195:THR:HG22	2.10	0.51
1:A:246:ALA:HB1	1:A:280:ILE:HD11	1.93	0.51
1:D:49:VAL:HG22	1:D:132:ARG:HD2	1.92	0.51
1:E:86:GLU:OE1	1:E:86:GLU:N	2.36	0.51
1:C:147:ALA:O	1:C:151:LYS:HG3	2.10	0.51
1:G:78:ALA:O	1:G:82:GLY:N	2.43	0.51
1:E:87:ASP:C	1:E:89:ALA:H	2.14	0.51
1:A:196:VAL:HG12	1:A:197:VAL:N	2.26	0.50
1:B:369:ARG:HH11	1:B:369:ARG:N	2.08	0.50
1:F:87:ASP:C	1:F:89:ALA:H	2.13	0.50
1:H:369:ARG:O	1:H:370:ASN:ND2	2.44	0.50
1:D:157:ALA:HA	1:D:160:MET:HE2	1.93	0.50
1:D:385:VAL:HG12	1:D:386:ARG:N	2.27	0.50
1:H:75:THR:O	1:H:79[B]:GLU:HG3	2.12	0.50
1:C:126:VAL:O	1:C:387:ARG:HD2	2.12	0.50
1:C:84:PRO:HD2	1:C:87:ASP:OD2	2.10	0.50
1:F:90:ASP:O	1:F:132:ARG:NH2	2.45	0.50
1:A:87:ASP:C	1:A:89:ALA:H	2.15	0.50
1:B:246:ALA:HB1	1:B:280:ILE:HD11	1.94	0.50
1:D:246:ALA:HB1	1:D:280:ILE:HD11	1.94	0.50
1:F:246:ALA:HB1	1:F:280:ILE:HD11	1.94	0.49
1:G:171:VAL:HG21	1:G:263:LEU:HD11	1.93	0.49
1:B:135:THR:CG2	1:B:151:LYS:HB3	2.41	0.49
1:H:246:ALA:HB1	1:H:280:ILE:HD11	1.94	0.49
1:G:303:CYS:SG	1:H:303:CYS:HB3	2.52	0.49
1:H:87:ASP:C	1:H:89:ALA:H	2.14	0.49
1:B:135:THR:HG22	1:B:136:GLU:O	2.12	0.49
1:C:346:LYS:NZ	2:C:402:HOH:O	2.45	0.49
1:B:369:ARG:HB2	1:B:369:ARG:NH1	2.29	0.48
1:C:270:SER:O	1:C:387:ARG:NH2	2.46	0.48
1:G:156:VAL:HG12	1:G:261:VAL:HG11	1.94	0.48
1:G:156:VAL:HG23	1:G:223:ALA:HB1	1.94	0.48
1:A:275:ARG:NH1	2:A:403:HOH:O	2.33	0.47
1:E:243:LEU:O	1:E:244:PHE:HD2	1.97	0.47
1:C:228:LYS:O	1:C:230:ASP:N	2.47	0.47
1:D:385:VAL:HG12	1:D:386:ARG:H	1.78	0.47
1:F:342[B]:HIS:CG	1:F:367:GLY:O	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:GLY:O	1:G:368:GLU:O	2.33	0.47
1:F:342[B]:HIS:CD2	1:F:367:GLY:O	2.67	0.47
1:G:22:VAL:C	1:G:23:VAL:CG2	2.83	0.47
1:D:49:VAL:HG22	1:D:132:ARG:CD	2.45	0.47
1:B:192:ARG:HA	1:F:301:PHE:O	2.15	0.46
1:F:188:ASP:O	1:F:191:SER:N	2.48	0.46
1:E:243:LEU:O	1:E:244:PHE:CD2	2.69	0.46
1:C:118:ASP:O	1:C:120:PRO:HD3	2.16	0.46
1:C:90:ASP:OD1	1:C:90:ASP:N	2.47	0.46
1:F:321:VAL:HG22	1:F:379:ASN:OD1	2.16	0.46
1:G:78:ALA:C	1:G:80:ALA:H	2.19	0.46
1:D:324:GLY:HA3	1:D:376:PRO:N	2.32	0.45
1:C:15:TYR:O	1:C:116:VAL:N	2.45	0.45
1:G:163:ALA:O	1:G:165:VAL:HG23	2.17	0.45
1:B:369:ARG:CB	1:B:369:ARG:HH11	2.29	0.45
1:G:131:GLY:HA2	1:G:162:ASP:OD2	2.17	0.45
1:F:16:PRO:HD2	1:F:269:GLN:O	2.16	0.45
1:A:321:VAL:HG22	1:A:379:ASN:OD1	2.17	0.44
1:G:370:ASN:HA	1:G:370:ASN:HD22	1.65	0.44
1:E:346:LYS:NZ	2:E:401:HOH:O	2.44	0.44
1:H:281:THR:O	1:H:378:GLY:HA2	2.18	0.44
1:H:369:ARG:HE	1:H:369:ARG:H	1.64	0.44
1:F:188:ASP:O	1:F:191:SER:HB2	2.17	0.44
1:G:281:THR:O	1:G:378:GLY:HA2	2.18	0.44
1:G:234:ASP:O	1:G:237:ILE:HG22	2.18	0.43
1:H:138:ILE:CD1	1:H:151:LYS:HD3	2.47	0.43
1:B:233:ALA:HB3	1:B:236:ARG:HG2	2.00	0.43
1:C:16:PRO:HD2	1:C:269:GLN:O	2.18	0.43
1:D:299:VAL:CG2	1:D:385:VAL:HG11	2.48	0.43
1:F:232:VAL:O	1:F:232:VAL:HG12	2.18	0.43
1:F:342[B]:HIS:CE1	1:F:367:GLY:O	2.71	0.43
1:F:195:THR:C	1:F:196:VAL:HG23	2.39	0.43
1:D:126:VAL:H	1:D:275:ARG:HH21	1.67	0.43
1:H:15:TYR:N	1:H:15:TYR:CD1	2.85	0.43
1:A:16:PRO:HD2	1:A:269:GLN:O	2.19	0.43
1:F:188:ASP:HA	1:F:191:SER:HB2	2.00	0.43
1:H:322:LEU:HD12	1:H:369:ARG:CG	2.47	0.43
1:H:35[B]:ARG:NH2	1:H:79[B]:GLU:OE2	2.51	0.43
1:D:16:PRO:HD2	1:D:269:GLN:O	2.19	0.42
1:F:194:LYS:C	1:F:195:THR:HG22	2.39	0.42
1:F:66:ARG:NH1	2:F:406:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:LEU:O	1:G:142:ASP:HB2	2.19	0.42
1:G:139:LEU:CB	1:G:141:GLU:HG3	2.48	0.42
1:A:85:VAL:HG12	1:A:86:GLU:OE2	2.20	0.42
1:A:209:MET:HG2	1:A:252:SER:OG	2.19	0.42
1:F:194:LYS:O	1:F:195:THR:CB	2.67	0.42
1:F:17:LYS:O	1:F:17:LYS:HG3	2.20	0.41
1:B:135:THR:HG21	1:B:138:ILE:HD11	2.02	0.41
1:F:189:ALA:O	1:F:194:LYS:CA	2.68	0.41
1:G:182:SER:O	1:G:186:VAL:HG23	2.19	0.41
1:B:369:ARG:HD3	1:B:369:ARG:N	2.35	0.41
1:E:16:PRO:HD2	1:E:269:GLN:O	2.21	0.41
1:H:16:PRO:HD2	1:H:269:GLN:O	2.20	0.41
1:G:139:LEU:HA	1:G:140:PRO:HD3	1.82	0.41
1:G:247:VAL:O	1:G:247:VAL:HG12	2.20	0.41
1:A:240:ASP:OD1	1:A:242:ASP:HB2	2.21	0.41
1:D:49:VAL:CG2	1:D:132:ARG:HD3	2.50	0.41
1:F:210:CYS:SG	1:F:211:TRP:CE3	3.10	0.41
1:E:281:THR:O	1:E:378:GLY:HA2	2.21	0.41
1:F:189:ALA:HB1	1:F:194:LYS:HA	2.02	0.41
1:D:312:GLN:HG2	1:D:385:VAL:HG12	2.03	0.41
1:F:210:CYS:SG	1:F:211:TRP:HE3	2.43	0.41
1:B:210:CYS:HB2	1:B:238:ARG:NH2	2.36	0.40
1:E:68:PHE:CD1	1:H:68:PHE:CD1	3.09	0.40
1:B:16:PRO:HD2	1:B:269:GLN:O	2.20	0.40
1:B:303:CYS:HB3	1:D:303:CYS:SG	2.61	0.40
1:F:281:THR:O	1:F:378:GLY:HA2	2.22	0.40
1:G:15:TYR:CB	1:G:16:PRO:CD	3.00	0.40
1:C:45:PRO:HB2	1:C:81:ARG:HG2	2.04	0.40
1:F:186:VAL:HG13	1:F:187:ALA:N	2.36	0.40

All (1) 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:B:234:ASP:OD1	1:E:193:GLY:O[4_445]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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	356/410 (87%)	343 (96%)	13 (4%)	0	100	100
1	B	354/410 (86%)	343 (97%)	10 (3%)	1 (0%)	46	68
1	C	342/410 (83%)	322 (94%)	18 (5%)	2 (1%)	30	52
1	D	327/410 (80%)	316 (97%)	11 (3%)	0	100	100
1	E	344/410 (84%)	335 (97%)	9 (3%)	0	100	100
1	F	341/410 (83%)	324 (95%)	13 (4%)	4 (1%)	16	30
1	G	329/410 (80%)	310 (94%)	15 (5%)	4 (1%)	16	30
1	H	320/410 (78%)	312 (98%)	8 (2%)	0	100	100
All	All	2713/3280 (83%)	2605 (96%)	97 (4%)	11 (0%)	39	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	80	ALA
1	C	88	LEU
1	G	141	GLU
1	G	368	GLU
1	B	368	GLU
1	F	195	THR
1	F	183	SER
1	G	88	LEU
1	F	368	GLU
1	G	16	PRO
1	F	376	PRO

5.3.2 Protein sidechains

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	263/310 (85%)	261 (99%)	2 (1%)	86	95
1	B	268/310 (86%)	266 (99%)	2 (1%)	88	96
1	C	241/310 (78%)	239 (99%)	2 (1%)	86	95
1	D	240/310 (77%)	237 (99%)	3 (1%)	76	90
1	E	254/310 (82%)	252 (99%)	2 (1%)	86	95
1	F	252/310 (81%)	246 (98%)	6 (2%)	57	80
1	G	241/310 (78%)	236 (98%)	5 (2%)	61	83
1	H	242/310 (78%)	238 (98%)	4 (2%)	68	86
All	All	2001/2480 (81%)	1975 (99%)	26 (1%)	76	90

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	PHE
1	A	303	CYS
1	B	303	CYS
1	B	369	ARG
1	C	177	LYS
1	C	303	CYS
1	D	92	VAL
1	D	211	TRP
1	D	303	CYS
1	E	231	LEU
1	E	303	CYS
1	F	119	LEU
1	F	188	ASP
1	F	211	TRP
1	F	235	ASP
1	F	282	ARG
1	F	303	CYS
1	G	141	GLU
1	G	229	ARG
1	G	272	SER
1	G	273	GLU
1	G	303	CYS
1	H	114	GLU
1	H	303	CYS

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Mol	Chain	Res	Type
1	H	369	ARG
1	H	370	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	134	HIS
1	G	172	HIS
1	G	370	ASN
1	H	370	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 carbohydrates 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

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	361/410 (88%)	0.16	20 (5%)	29	26	19, 41, 99, 140	0
1	B	360/410 (87%)	0.14	14 (3%)	43	40	22, 47, 86, 130	0
1	C	348/410 (84%)	0.31	19 (5%)	29	26	20, 57, 107, 144	0
1	D	333/410 (81%)	0.46	21 (6%)	23	21	24, 58, 106, 134	0
1	E	349/410 (85%)	0.13	13 (3%)	45	42	20, 42, 105, 137	0
1	F	350/410 (85%)	0.38	28 (8%)	15	13	22, 48, 99, 122	0
1	G	340/410 (82%)	0.78	50 (14%)	3	2	25, 70, 111, 138	0
1	H	328/410 (80%)	0.25	22 (6%)	21	19	22, 49, 95, 139	0
All	All	2769/3280 (84%)	0.32	187 (6%)	20	18	19, 51, 104, 144	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ILE	7.9
1	F	235	ASP	7.5
1	F	191	SER	7.0
1	D	235	ASP	6.3
1	H	211	TRP	6.3
1	G	233	ALA	6.2
1	D	232	VAL	6.0
1	F	187	ALA	5.9
1	F	233	ALA	5.9
1	F	146	THR	5.8
1	D	233	ALA	5.7
1	F	232	VAL	5.6
1	H	147	ALA	5.4
1	A	390	ALA	5.4
1	E	183	SER	5.3
1	F	230	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	H	148	GLN	4.9
1	G	218	LEU	4.8
1	A	235	ASP	4.8
1	D	234	ASP	4.8
1	C	211	TRP	4.7
1	D	146	THR	4.4
1	G	47	SER	4.4
1	E	195	THR	4.3
1	H	195	THR	4.2
1	F	227	VAL	4.2
1	E	185	ALA	4.2
1	H	218	LEU	4.1
1	H	138	ILE	4.0
1	G	133	GLY	3.9
1	G	211	TRP	3.9
1	D	119	LEU	3.9
1	H	210	CYS	3.9
1	F	218	LEU	3.9
1	A	146	THR	3.8
1	B	146	THR	3.7
1	G	138	ILE	3.7
1	D	211	TRP	3.7
1	H	215	ALA	3.7
1	B	243	LEU	3.7
1	H	227	VAL	3.6
1	E	187	ALA	3.6
1	F	234	ASP	3.6
1	A	243	LEU	3.6
1	D	139	LEU	3.5
1	F	185	ALA	3.5
1	B	147	ALA	3.5
1	F	211	TRP	3.5
1	G	235	ASP	3.5
1	H	145	ARG	3.5
1	G	194	LYS	3.5
1	F	231	LEU	3.4
1	F	152	VAL	3.4
1	F	190	LEU	3.4
1	D	114	GLU	3.4
1	H	146	THR	3.3
1	A	239	SER	3.3
1	G	180	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	115	TRP	3.3
1	D	88	LEU	3.3
1	C	126	VAL	3.2
1	E	181	LEU	3.2
1	E	230	ASP	3.2
1	F	142	ASP	3.2
1	A	191	SER	3.2
1	A	185	ALA	3.1
1	E	231	LEU	3.1
1	F	147	ALA	3.1
1	E	209	MET	3.1
1	G	44	ASP	3.0
1	C	193	GLY	3.0
1	F	149	VAL	3.0
1	D	230	ASP	3.0
1	F	144	GLY	3.0
1	A	240	ASP	3.0
1	F	245	SER	3.0
1	D	123	LEU	3.0
1	D	181	LEU	3.0
1	C	138	ILE	3.0
1	F	188	ASP	3.0
1	D	147	ALA	3.0
1	E	186	VAL	2.9
1	A	234	ASP	2.9
1	C	119	LEU	2.9
1	C	187	ALA	2.9
1	G	112	THR	2.9
1	G	193	GLY	2.9
1	G	73	LEU	2.9
1	D	231	LEU	2.9
1	F	181	LEU	2.9
1	A	187	ALA	2.8
1	B	232	VAL	2.8
1	C	244	PHE	2.8
1	G	210	CYS	2.8
1	B	367	GLY	2.8
1	B	236	ARG	2.8
1	D	180	ALA	2.8
1	G	234	ASP	2.8
1	G	88	LEU	2.8
1	A	145	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	244	PHE	2.8
1	H	208	SER	2.8
1	H	253	GLY	2.8
1	G	40	SER	2.7
1	G	45	PRO	2.7
1	D	76	ALA	2.7
1	C	144	GLY	2.7
1	E	125	GLY	2.7
1	H	367	GLY	2.7
1	H	220	VAL	2.7
1	H	149	VAL	2.7
1	C	216	SER	2.7
1	G	179	PRO	2.7
1	H	219	GLY	2.6
1	C	145	ARG	2.6
1	G	85	VAL	2.6
1	A	218	LEU	2.6
1	G	161	LEU	2.6
1	C	227	VAL	2.5
1	G	87	ASP	2.5
1	C	143	ILE	2.5
1	G	91	SER	2.5
1	A	233	ALA	2.5
1	G	46	ALA	2.5
1	F	222	VAL	2.5
1	G	268	ALA	2.5
1	G	237	ILE	2.4
1	G	244	PHE	2.4
1	B	231	LEU	2.4
1	C	181	LEU	2.4
1	A	211	TRP	2.4
1	G	219	GLY	2.4
1	H	144	GLY	2.4
1	A	230	ASP	2.4
1	B	237	ILE	2.4
1	G	255	GLU	2.4
1	B	225	GLY	2.4
1	A	150	ASP	2.4
1	G	145	ARG	2.4
1	E	182	SER	2.4
1	G	131	GLY	2.3
1	D	210	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	236	ARG	2.3
1	G	248	ALA	2.3
1	C	255	GLU	2.3
1	G	48	VAL	2.3
1	B	234	ASP	2.3
1	A	232	VAL	2.3
1	G	164	GLY	2.3
1	G	215	ALA	2.2
1	C	148	GLN	2.2
1	A	90	ASP	2.2
1	H	254	GLY	2.2
1	B	233	ALA	2.2
1	G	34	PHE	2.2
1	B	235	ASP	2.2
1	C	139	LEU	2.2
1	D	144	GLY	2.2
1	A	195	THR	2.2
1	E	123	LEU	2.2
1	C	146	THR	2.1
1	H	115	TRP	2.1
1	G	228	LYS	2.1
1	D	227	VAL	2.1
1	F	192	ARG	2.1
1	G	43	VAL	2.1
1	G	185	ALA	2.1
1	H	143	ILE	2.1
1	C	183	SER	2.1
1	G	242	ASP	2.1
1	G	300	ASP	2.1
1	G	22	VAL	2.1
1	G	42	ALA	2.1
1	G	132	ARG	2.1
1	G	217	ALA	2.1
1	H	196	VAL	2.1
1	G	209	MET	2.0
1	D	89	ALA	2.0
1	G	92	VAL	2.0
1	G	232	VAL	2.0
1	G	378	GLY	2.0
1	E	184	ARG	2.0
1	G	166	THR	2.0
1	F	183	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	150	ASP	2.0
1	F	228	LYS	2.0
1	C	209	MET	2.0

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.