Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:52 pm BST

PDB ID	:	4L8Y
Title	:	Crystal structure of gamma-glutamyl hydrolase (C108A) from zebrafish
Authors	:	Chuankhayan, P.; Kao, T.-T.; Chen, C.-J.; Fu, T.-F.
Deposited on	:	2013-06-18
Resolution	:	1.97 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

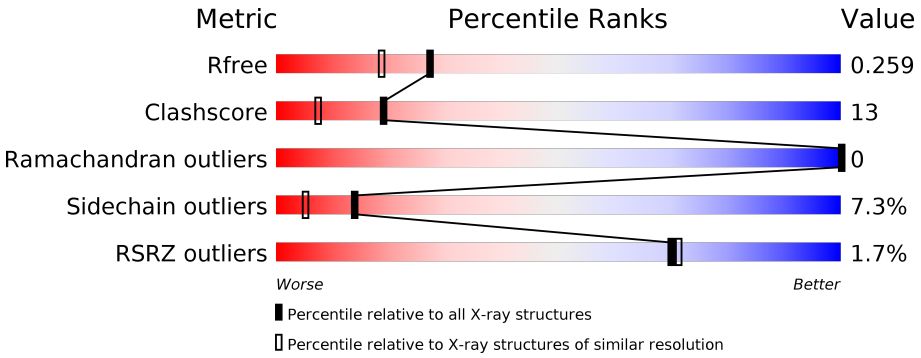
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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	312	3% 76% 12% • 8%
1	B	312	71% 17% • • 8%
1	C	312	2% 71% 16% • • 8%
1	D	312	% 67% 20% • • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10096 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 Gamma-glutamyl hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	287	Total	C	N	O	S	0	0	0
			2308	1492	370	442	4			
1	D	287	Total	C	N	O	S	0	0	0
			2308	1492	370	442	4			
1	A	287	Total	C	N	O	S	0	0	0
			2308	1492	370	442	4			
1	B	287	Total	C	N	O	S	0	0	0
			2308	1492	370	442	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	108	ALA	CYS	ENGINEERED MUTATION	UNP Q6NY42
D	108	ALA	CYS	ENGINEERED MUTATION	UNP Q6NY42
A	108	ALA	CYS	ENGINEERED MUTATION	UNP Q6NY42
B	108	ALA	CYS	ENGINEERED MUTATION	UNP Q6NY42

- Molecule 2 is water.

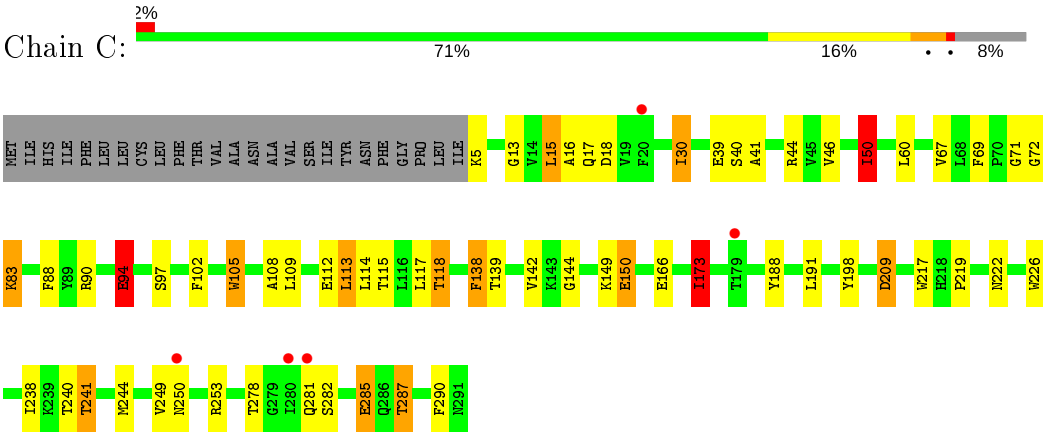
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	225	Total	O	0	0
			225	225		
2	D	270	Total	O	0	0
			270	270		
2	A	192	Total	O	0	0
			192	192		
2	B	177	Total	O	0	0
			177	177		

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 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.

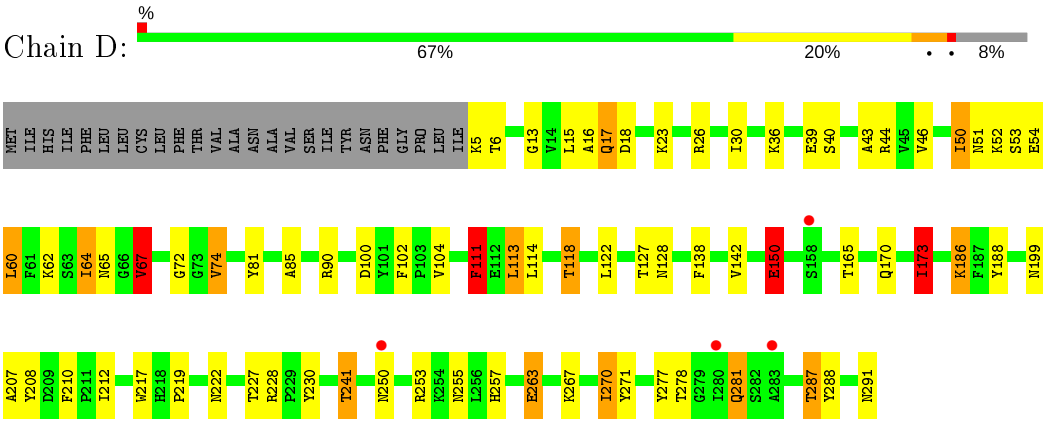
- Molecule 1: Gamma-glutamyl hydrolase

Chain C:



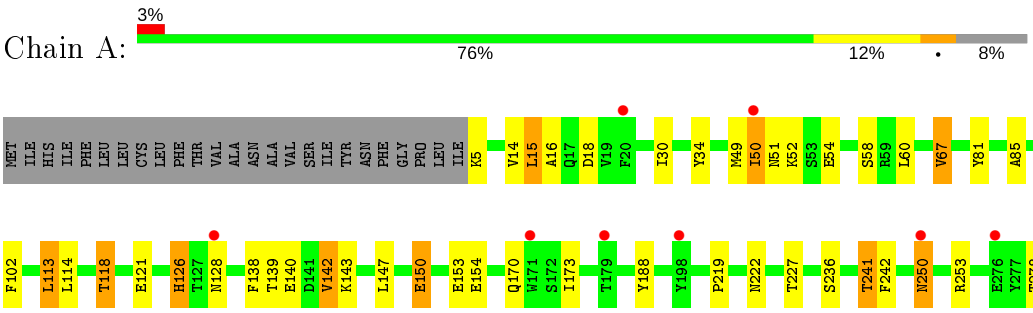
- Molecule 1: Gamma-glutamyl hydrolase

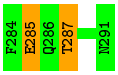
Chain D:



- Molecule 1: Gamma-glutamyl hydrolase

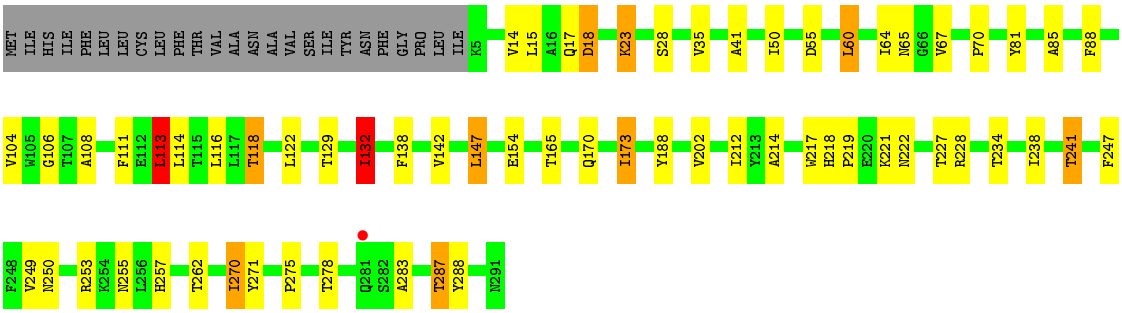
Chain A:





• Molecule 1: Gamma-glutamyl hydrolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.59Å 206.50Å 65.20Å 90.00° 113.42° 90.00°	Depositor
Resolution (Å)	30.00 – 1.97 29.91 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-1.97) 99.1 (29.91-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.258 0.200 , 0.259	Depositor DCC
R_{free} test set	4361 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 14.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10096	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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	1.09	3/2373 (0.1%)	0.93	3/3220 (0.1%)
1	B	1.05	2/2373 (0.1%)	0.97	3/3220 (0.1%)
1	C	1.27	9/2373 (0.4%)	1.03	8/3220 (0.2%)
1	D	1.21	10/2373 (0.4%)	1.04	10/3220 (0.3%)
All	All	1.16	24/9492 (0.3%)	0.99	24/12880 (0.2%)

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	C	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	150	GLU	CD-OE1	9.58	1.36	1.25
1	D	74	VAL	CB-CG1	-6.91	1.38	1.52
1	C	226	TRP	CZ3-CH2	6.75	1.50	1.40
1	A	150	GLU	CD-OE1	6.67	1.32	1.25
1	D	208	TYR	CD2-CE2	6.38	1.49	1.39
1	C	217	TRP	CE3-CZ3	5.99	1.48	1.38
1	D	111	PHE	CE2-CZ	5.96	1.48	1.37
1	B	154	GLU	CB-CG	5.95	1.63	1.52
1	A	34	TYR	CE1-CZ	5.80	1.46	1.38
1	D	81	TYR	CD1-CE1	5.79	1.48	1.39
1	D	51	ASN	N-CA	5.70	1.57	1.46
1	C	105	TRP	CE3-CZ3	5.66	1.48	1.38
1	C	94	GLU	CG-CD	-5.61	1.43	1.51
1	D	17	GLN	CB-CG	-5.58	1.37	1.52
1	C	198	TYR	CD1-CE1	5.58	1.47	1.39
1	C	150	GLU	CD-OE2	5.57	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	PHE	CE1-CZ	5.42	1.47	1.37
1	B	14	VAL	CB-CG1	5.40	1.64	1.52
1	D	201	PHE	CG-CD1	5.31	1.46	1.38
1	A	242	PHE	CE1-CZ	5.10	1.47	1.37
1	D	277	TYR	CE1-CZ	5.09	1.45	1.38
1	C	198	TYR	CE1-CZ	5.08	1.45	1.38
1	D	150	GLU	CD-OE1	5.04	1.31	1.25
1	D	150	GLU	CG-CD	5.01	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	132	ILE	CB-CA-C	-8.50	94.59	111.60
1	D	67	VAL	CG1-CB-CG2	8.35	124.27	110.90
1	C	44	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	C	50	ILE	C-N-CA	-8.03	101.64	121.70
1	C	173	ILE	CB-CA-C	-7.57	96.46	111.60
1	A	67	VAL	CG1-CB-CG2	-7.57	98.79	110.90
1	D	44	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	D	100	ASP	CB-CG-OD1	7.02	124.61	118.30
1	C	44	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	116	LEU	CA-CB-CG	6.40	130.01	115.30
1	D	50	ILE	C-N-CA	-6.26	106.05	121.70
1	D	173	ILE	CB-CA-C	-6.24	99.12	111.60
1	D	67	VAL	CB-CA-C	-6.03	99.95	111.40
1	D	44	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	C	97	SER	CB-CA-C	5.49	120.53	110.10
1	B	113	LEU	CA-CB-CG	5.46	127.86	115.30
1	D	15	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	D	67	VAL	CA-CB-CG1	5.34	118.90	110.90
1	C	209	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	17	GLN	N-CA-CB	-5.15	101.32	110.60
1	A	15	LEU	CB-CG-CD2	-5.13	102.27	111.00
1	C	240	THR	CA-CB-CG2	-5.12	105.23	112.40
1	C	30	ILE	CB-CA-C	-5.05	101.50	111.60
1	A	236	SER	CB-CA-C	5.05	119.69	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	144	GLY	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	2308	0	2229	62	0
1	B	2308	0	2229	47	0
1	C	2308	0	2229	62	0
1	D	2308	0	2229	88	0
2	A	192	0	0	10	0
2	B	177	0	0	1	0
2	C	225	0	0	7	0
2	D	270	0	0	23	0
All	All	10096	0	8916	235	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 13.

All (235) 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:D:40:SER:HB2	2:D:322:HOH:O	1.34	1.26
1:D:90:ARG:HD3	2:D:312:HOH:O	1.35	1.25
1:C:83:LYS:NZ	1:C:83:LYS:HB3	1.65	1.11
1:C:94:GLU:HG2	2:C:365:HOH:O	1.52	1.09
1:C:115:THR:HG21	1:C:173:ILE:CD1	1.86	1.05
1:D:90:ARG:CD	2:D:312:HOH:O	1.91	1.05
1:A:100:ASP:HB2	2:A:334:HOH:O	1.57	1.04
1:A:222:ASN:HB2	1:A:241:THR:CG2	1.87	1.03
1:C:285:GLU:HG2	1:D:271:TYR:CE1	1.95	1.00
1:D:230:TYR:OH	1:A:128:ASN:ND2	1.94	1.00
1:D:50:ILE:HG12	2:D:351:HOH:O	1.62	0.97
1:D:50:ILE:HG21	2:D:351:HOH:O	1.63	0.96
1:C:287:THR:HG21	2:C:499:HOH:O	1.68	0.93
1:C:115:THR:HG21	1:C:173:ILE:HD11	1.48	0.92
1:C:83:LYS:HZ2	1:C:83:LYS:HB3	1.26	0.91
1:D:270:ILE:HD11	1:D:288:TYR:CE2	2.08	0.88
1:D:222:ASN:HB2	1:D:241:THR:CG2	2.05	0.87
1:B:227:THR:HG23	1:B:228:ARG:HG2	1.58	0.85
1:C:83:LYS:NZ	1:C:83:LYS:CB	2.37	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ILE:HD13	1:D:270:ILE:O	1.76	0.85
1:C:115:THR:HG21	1:C:173:ILE:HD12	1.58	0.84
1:B:129:THR:HA	1:B:132:ILE:HD11	1.62	0.82
1:A:222:ASN:HB2	1:A:241:THR:HG22	1.62	0.81
1:D:53:SER:OG	1:D:56:GLU:HG3	1.82	0.80
1:D:90:ARG:NH2	2:D:545:HOH:O	2.14	0.80
1:A:227:THR:HG23	1:A:285:GLU:OE1	1.82	0.80
1:A:54:GLU:OE2	2:A:467:HOH:O	1.99	0.79
1:B:65:ASN:HD22	1:B:255:ASN:HD22	1.28	0.79
1:A:219:PRO:O	1:A:241:THR:HB	1.83	0.78
1:B:23:LYS:HA	1:B:23:LYS:HE3	1.63	0.78
1:C:83:LYS:HZ3	1:C:83:LYS:HB3	1.47	0.78
1:D:170:GLN:HG2	1:A:126:HIS:CE1	2.19	0.77
1:C:278:THR:HG21	1:C:287:THR:HG23	1.68	0.76
1:C:222:ASN:HB2	1:C:241:THR:CG2	2.17	0.75
1:A:50:ILE:HD11	1:A:81:TYR:HA	1.67	0.75
1:B:219:PRO:O	1:B:241:THR:HB	1.87	0.75
1:D:65:ASN:HD22	1:D:255:ASN:HD22	1.33	0.75
1:C:83:LYS:HZ2	1:C:83:LYS:CB	1.96	0.74
1:A:140:GLU:OE1	1:A:143:LYS:NZ	2.21	0.74
1:A:139:THR:O	1:A:142:VAL:HG22	1.87	0.73
1:C:30:ILE:HG12	1:C:290:PHE:HE1	1.53	0.73
1:D:255:ASN:ND2	1:D:257:HIS:H	1.86	0.73
1:B:18:ASP:OD2	1:B:50:ILE:HD11	1.89	0.72
1:C:16:ALA:HA	1:C:30:ILE:HD13	1.72	0.71
1:C:94:GLU:OE1	2:C:365:HOH:O	2.08	0.71
1:B:222:ASN:HB2	1:B:241:THR:CG2	2.21	0.71
1:A:280:ILE:H	1:A:280:ILE:HD12	1.53	0.71
1:C:50:ILE:HD11	1:C:81:TYR:HA	1.72	0.71
1:D:287:THR:HG21	2:D:565:HOH:O	1.90	0.70
1:B:227:THR:HG21	1:B:283:ALA:O	1.94	0.68
1:B:270:ILE:HD11	1:B:288:TYR:CZ	2.28	0.68
1:B:222:ASN:HB2	1:B:241:THR:HG22	1.77	0.67
1:D:104:VAL:HB	1:D:212:ILE:HD12	1.76	0.67
1:D:170:GLN:HE21	1:A:126:HIS:CG	2.13	0.67
1:A:173:ILE:HG23	1:A:173:ILE:O	1.93	0.67
1:D:170:GLN:HE21	1:A:126:HIS:CB	2.09	0.66
1:C:67:VAL:HG23	1:C:102:PHE:CZ	2.31	0.65
1:D:278:THR:HG21	1:D:287:THR:HG23	1.79	0.64
1:D:219:PRO:O	1:D:241:THR:HB	1.97	0.64
1:C:105:TRP:HH2	1:C:244:MET:HE3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:PHE:CD2	1:B:142:VAL:HG11	2.32	0.63
1:A:253:ARG:NH2	1:B:238:ILE:HD13	2.14	0.63
1:D:170:GLN:HE21	1:A:126:HIS:HB2	1.63	0.63
1:A:5:LYS:NZ	1:A:5:LYS:HB3	2.13	0.62
1:A:100:ASP:CB	2:A:334:HOH:O	2.28	0.62
1:D:230:TYR:OH	1:A:128:ASN:CG	2.37	0.62
1:B:255:ASN:ND2	1:B:257:HIS:H	1.96	0.62
1:C:30:ILE:HG12	1:C:290:PHE:CE1	2.34	0.62
1:D:222:ASN:HB2	1:D:241:THR:HG22	1.82	0.62
1:D:270:ILE:HD12	2:D:372:HOH:O	2.02	0.60
1:D:255:ASN:HD21	1:D:257:HIS:CG	2.20	0.60
1:A:85:ALA:HB3	1:A:113:LEU:HD11	1.84	0.60
1:D:50:ILE:CG2	2:D:351:HOH:O	2.35	0.60
1:C:114:LEU:O	1:C:118:THR:HG23	2.02	0.59
1:D:291:ASN:OXT	2:D:532:HOH:O	2.17	0.59
1:C:219:PRO:O	1:C:241:THR:HB	2.03	0.58
1:B:104:VAL:HB	1:B:212:ILE:CD1	2.32	0.58
1:A:138:PHE:CD2	1:A:142:VAL:HG11	2.38	0.58
1:D:150:GLU:HG3	2:D:392:HOH:O	2.03	0.58
1:C:118:THR:HG21	1:C:188:TYR:OH	2.03	0.58
1:D:150:GLU:CG	2:D:392:HOH:O	2.52	0.58
1:A:250:ASN:HB3	2:A:306:HOH:O	2.03	0.58
1:D:138:PHE:CD2	1:D:142:VAL:HG11	2.38	0.58
1:D:270:ILE:CD1	1:D:288:TYR:CE2	2.85	0.58
1:B:255:ASN:HD21	1:B:257:HIS:CG	2.22	0.57
1:B:41:ALA:HB3	1:B:249:VAL:HG21	1.85	0.57
1:D:230:TYR:CE2	1:A:128:ASN:ND2	2.69	0.57
1:D:263:GLU:HG2	2:D:359:HOH:O	2.03	0.57
1:A:285:GLU:HG3	1:B:271:TYR:CE1	2.41	0.56
1:D:270:ILE:HD11	1:D:288:TYR:CZ	2.39	0.56
1:C:278:THR:CG2	1:C:287:THR:HG23	2.34	0.56
1:A:30:ILE:HD13	2:A:323:HOH:O	2.06	0.56
1:A:14:VAL:HG12	1:A:30:ILE:HD12	1.86	0.56
1:B:114:LEU:O	1:B:118:THR:HG23	2.06	0.56
1:C:67:VAL:HG23	1:C:102:PHE:HZ	1.72	0.55
1:C:285:GLU:HG2	1:D:271:TYR:CZ	2.41	0.55
1:C:105:TRP:CH2	1:C:244:MET:HE3	2.42	0.55
1:D:60:LEU:O	1:D:64:ILE:HD12	2.07	0.54
1:A:222:ASN:HB2	1:A:241:THR:HG21	1.81	0.54
1:C:16:ALA:HA	1:C:30:ILE:CD1	2.38	0.54
1:A:100:ASP:CG	2:A:334:HOH:O	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLU:CG	2:C:365:HOH:O	2.28	0.54
1:D:267:LYS:HD3	2:D:362:HOH:O	2.07	0.54
1:D:170:GLN:NE2	1:A:126:HIS:HB2	2.22	0.53
1:C:142:VAL:CG1	1:C:191:LEU:O	2.56	0.53
1:D:111:PHE:CZ	1:D:173:ILE:HD11	2.43	0.53
1:B:104:VAL:HB	1:B:212:ILE:HD12	1.90	0.53
1:C:166:GLU:HG3	1:C:231:ILE:HD12	1.91	0.53
1:A:15:LEU:C	1:A:30:ILE:HD11	2.29	0.52
1:A:114:LEU:O	1:A:118:THR:HG23	2.09	0.52
1:D:90:ARG:CZ	2:D:566:HOH:O	2.57	0.52
1:D:118:THR:HG21	1:D:188:TYR:OH	2.10	0.52
1:C:285:GLU:CG	1:D:271:TYR:CE1	2.84	0.52
1:D:127:THR:O	1:A:170:GLN:NE2	2.43	0.52
1:D:65:ASN:HD22	1:D:255:ASN:ND2	2.03	0.52
1:A:16:ALA:O	1:A:50:ILE:HD13	2.10	0.52
1:C:115:THR:CG2	1:C:173:ILE:HD11	2.33	0.51
1:D:228:ARG:HB3	1:D:230:TYR:CE2	2.45	0.51
1:D:52:LYS:HB2	1:D:57:TYR:CZ	2.45	0.51
1:D:54:GLU:HB2	2:D:352:HOH:O	2.10	0.51
1:D:170:GLN:NE2	1:A:126:HIS:CG	2.78	0.51
1:C:90:ARG:NH2	2:C:414:HOH:O	2.44	0.51
1:D:230:TYR:OH	1:A:128:ASN:OD1	2.27	0.51
1:D:278:THR:CG2	1:D:287:THR:HG23	2.39	0.51
1:D:111:PHE:HZ	1:D:173:ILE:HD11	1.75	0.51
1:C:67:VAL:HG21	1:C:88:PHE:CD2	2.46	0.51
1:A:67:VAL:HG23	1:A:102:PHE:HZ	1.75	0.51
1:A:50:ILE:HD11	1:A:81:TYR:CA	2.38	0.50
1:C:142:VAL:HG12	1:C:191:LEU:O	2.11	0.50
1:D:170:GLN:HG2	1:A:126:HIS:CG	2.46	0.50
1:A:16:ALA:N	1:A:30:ILE:HD11	2.27	0.50
1:A:250:ASN:CB	2:A:306:HOH:O	2.60	0.50
1:C:15:LEU:HD12	1:C:69:PHE:CD2	2.47	0.50
1:A:118:THR:HG21	1:A:188:TYR:OH	2.12	0.50
1:C:17:GLN:OE1	1:C:72:GLY:HA3	2.12	0.49
1:D:222:ASN:HB2	1:D:241:THR:HG21	1.92	0.49
1:D:250:ASN:ND2	1:D:253:ARG:HH11	2.11	0.49
1:A:285:GLU:OE1	1:A:285:GLU:CA	2.59	0.49
1:D:46:VAL:HG13	2:D:539:HOH:O	2.11	0.49
1:B:222:ASN:HB2	1:B:241:THR:HG21	1.93	0.49
1:A:49:MET:HB2	1:A:52:LYS:HE3	1.93	0.49
1:C:228:ARG:O	1:C:231:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:THR:HG21	1:B:287:THR:HG23	1.95	0.49
1:A:173:ILE:O	1:A:173:ILE:CG2	2.61	0.48
1:D:170:GLN:HG2	1:A:126:HIS:CD2	2.49	0.48
1:D:50:ILE:CB	2:D:351:HOH:O	2.58	0.48
1:D:16:ALA:HA	1:D:30:ILE:HG13	1.96	0.48
1:D:111:PHE:CD2	1:D:111:PHE:C	2.86	0.48
1:B:118:THR:HG21	1:B:188:TYR:OH	2.14	0.47
1:C:139:THR:O	1:C:142:VAL:HG13	2.14	0.47
1:C:41:ALA:HB3	1:C:249:VAL:HG21	1.96	0.47
1:C:83:LYS:NZ	2:C:508:HOH:O	2.14	0.47
1:C:108:ALA:O	1:C:112:GLU:HG3	2.14	0.47
1:A:51:ASN:N	2:A:471:HOH:O	1.93	0.47
1:B:147:LEU:HD23	1:B:247:PHE:CD2	2.48	0.47
1:D:170:GLN:HG2	1:A:126:HIS:ND1	2.29	0.47
1:C:118:THR:CG2	1:C:188:TYR:OH	2.63	0.47
1:D:207:ALA:HB3	1:D:210:PHE:O	2.15	0.47
1:C:39:GLU:OE1	1:D:36:LYS:NZ	2.48	0.47
1:D:173:ILE:O	1:D:173:ILE:HD12	2.15	0.46
1:C:50:ILE:HG13	1:C:80:GLY:HA3	1.97	0.46
1:D:170:GLN:NE2	1:A:126:HIS:CD2	2.84	0.46
1:B:234:THR:O	1:B:238:ILE:HD12	2.16	0.46
1:C:278:THR:OG1	1:C:287:THR:HG22	2.16	0.46
1:B:108:ALA:O	1:B:111:PHE:HB3	2.16	0.46
1:D:278:THR:OG1	1:D:287:THR:CG2	2.63	0.46
1:A:94:GLU:HG2	2:A:313:HOH:O	2.16	0.45
1:A:16:ALA:HA	1:A:30:ILE:CD1	2.46	0.45
1:C:67:VAL:HG23	1:C:102:PHE:CE2	2.52	0.45
1:D:118:THR:CG2	1:D:188:TYR:OH	2.65	0.45
1:D:173:ILE:CD1	1:D:202:VAL:HB	2.46	0.45
1:A:5:LYS:HB3	1:A:5:LYS:HZ3	1.81	0.45
1:D:170:GLN:HG2	1:A:126:HIS:NE2	2.31	0.45
1:C:278:THR:HG21	1:C:287:THR:CG2	2.41	0.45
1:A:283:ALA:HB2	2:A:417:HOH:O	2.17	0.44
1:A:278:THR:OG1	1:A:287:THR:HG23	2.18	0.44
1:D:270:ILE:HD13	1:D:270:ILE:C	2.37	0.44
1:D:270:ILE:CD1	1:D:270:ILE:O	2.59	0.44
1:D:64:ILE:C	1:D:64:ILE:HD13	2.37	0.44
1:A:85:ALA:CB	1:A:113:LEU:CD1	2.96	0.44
1:A:253:ARG:HH22	1:B:238:ILE:HD13	1.82	0.44
1:A:219:PRO:O	1:A:241:THR:CG2	2.65	0.44
1:C:222:ASN:HB2	1:C:241:THR:HG21	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLY:HA2	1:C:46:VAL:O	2.18	0.44
1:D:281:GLN:HB2	2:D:348:HOH:O	2.18	0.44
1:C:50:ILE:HD12	1:C:50:ILE:HA	1.50	0.44
1:D:165:THR:HB	1:D:217:TRP:CE3	2.53	0.44
1:B:106:GLY:O	1:B:214:ALA:HA	2.18	0.44
1:C:138:PHE:HB3	1:C:142:VAL:HG11	2.00	0.44
1:C:105:TRP:HH2	1:C:244:MET:CE	2.30	0.43
1:D:114:LEU:O	1:D:118:THR:HG23	2.18	0.43
1:D:67:VAL:HG22	1:D:102:PHE:HE2	1.82	0.43
1:D:17:GLN:OE1	1:D:72:GLY:HA3	2.19	0.43
1:B:85:ALA:HB3	1:B:113:LEU:HD11	2.01	0.43
1:D:39:GLU:HA	1:D:43:ALA:O	2.19	0.43
1:A:126:HIS:CE1	1:A:170:GLN:HB2	2.53	0.43
1:C:149:LYS:HE2	2:C:378:HOH:O	2.18	0.43
1:D:90:ARG:NE	2:D:566:HOH:O	2.51	0.43
1:B:218:HIS:HB3	1:B:221:LYS:HG3	2.01	0.43
1:C:71:GLY:HA2	1:C:109:LEU:HB3	2.00	0.43
1:D:13:GLY:HA2	1:D:46:VAL:O	2.18	0.43
1:D:104:VAL:HB	1:D:212:ILE:CD1	2.46	0.42
1:B:218:HIS:CG	1:B:221:LYS:HE2	2.54	0.42
1:D:186:LYS:CD	2:D:355:HOH:O	2.67	0.42
1:C:40:SER:OG	1:D:40:SER:OG	2.31	0.42
1:B:138:PHE:HB3	1:B:142:VAL:HG11	2.00	0.42
1:B:275:PRO:HD3	1:B:288:TYR:CE2	2.54	0.42
1:B:67:VAL:HG11	1:B:88:PHE:CD2	2.54	0.42
1:C:250:ASN:ND2	1:C:253:ARG:HH11	2.18	0.42
1:C:50:ILE:HG13	1:C:80:GLY:C	2.40	0.42
1:C:90:ARG:HD2	1:C:90:ARG:HH11	1.71	0.42
1:B:173:ILE:CD1	1:B:202:VAL:HB	2.50	0.42
1:B:35:VAL:HG11	1:B:270:ILE:HD12	2.02	0.42
1:B:65:ASN:HD22	1:B:255:ASN:ND2	2.07	0.42
1:C:113:LEU:HD13	1:C:117:LEU:HD11	2.00	0.42
1:A:16:ALA:HA	1:A:30:ILE:HD11	2.02	0.41
1:C:50:ILE:HD11	1:C:81:TYR:CA	2.44	0.41
1:D:26:ARG:O	1:D:26:ARG:HG2	2.19	0.41
1:B:270:ILE:HD13	2:B:450:HOH:O	2.20	0.41
1:D:227:THR:HG22	2:D:458:HOH:O	2.20	0.41
1:D:62:LYS:O	1:D:257:HIS:HB3	2.20	0.41
1:D:85:ALA:HB3	1:D:113:LEU:HD11	2.03	0.41
1:B:250:ASN:ND2	1:B:253:ARG:HH11	2.19	0.41
1:B:173:ILE:HD12	1:B:202:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PRO:HD2	1:B:81:TYR:HE1	1.86	0.41
1:B:118:THR:HG21	1:B:188:TYR:CE2	2.55	0.41
1:B:165:THR:HB	1:B:217:TRP:CE3	2.55	0.41
1:B:104:VAL:HB	1:B:212:ILE:HD13	2.01	0.41
1:B:18:ASP:OD2	1:B:50:ILE:CD1	2.65	0.41
1:B:60:LEU:HD22	1:B:64:ILE:CG2	2.50	0.41
1:D:5:LYS:N	2:D:315:HOH:O	2.54	0.41
1:B:17:GLN:O	1:B:28:SER:HA	2.21	0.40
1:A:67:VAL:HG23	1:A:102:PHE:CZ	2.56	0.40
1:B:60:LEU:HD22	1:B:64:ILE:HG23	2.03	0.40
1:A:50:ILE:HD12	1:A:50:ILE:HA	1.68	0.40

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	285/312 (91%)	275 (96%)	10 (4%)	0	100	100
1	B	285/312 (91%)	274 (96%)	11 (4%)	0	100	100
1	C	285/312 (91%)	279 (98%)	6 (2%)	0	100	100
1	D	285/312 (91%)	277 (97%)	8 (3%)	0	100	100
All	All	1140/1248 (91%)	1105 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	249/271 (92%)	231 (93%)	18 (7%)	14 5
1	B	249/271 (92%)	233 (94%)	16 (6%)	17 7
1	C	249/271 (92%)	231 (93%)	18 (7%)	14 5
1	D	249/271 (92%)	228 (92%)	21 (8%)	11 2
All	All	996/1084 (92%)	923 (93%)	73 (7%)	14 5

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	LYS
1	C	15	LEU
1	C	18	ASP
1	C	50	ILE
1	C	60	LEU
1	C	83	LYS
1	C	94	GLU
1	C	113	LEU
1	C	118	THR
1	C	150	GLU
1	C	173	ILE
1	C	209	ASP
1	C	238	ILE
1	C	241	THR
1	C	281	GLN
1	C	282	SER
1	C	285	GLU
1	C	287	THR
1	D	6	THR
1	D	18	ASP
1	D	23	LYS
1	D	60	LEU
1	D	64	ILE
1	D	67	VAL
1	D	74	VAL
1	D	111	PHE
1	D	113	LEU
1	D	118	THR
1	D	122	LEU
1	D	128	ASN

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Mol	Chain	Res	Type
1	D	150	GLU
1	D	173	ILE
1	D	186	LYS
1	D	199	ASN
1	D	241	THR
1	D	263	GLU
1	D	270	ILE
1	D	281	GLN
1	D	287	THR
1	A	18	ASP
1	A	50	ILE
1	A	58	SER
1	A	60	LEU
1	A	94	GLU
1	A	113	LEU
1	A	118	THR
1	A	121	GLU
1	A	126	HIS
1	A	142	VAL
1	A	147	LEU
1	A	150	GLU
1	A	153	GLU
1	A	154	GLU
1	A	241	THR
1	A	250	ASN
1	A	285	GLU
1	A	287	THR
1	B	15	LEU
1	B	18	ASP
1	B	23	LYS
1	B	55	ASP
1	B	60	LEU
1	B	113	LEU
1	B	118	THR
1	B	122	LEU
1	B	132	ILE
1	B	147	LEU
1	B	170	GLN
1	B	173	ILE
1	B	241	THR
1	B	262	THR
1	B	270	ILE

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Mol	Chain	Res	Type
1	B	287	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	167	ASN
1	C	250	ASN
1	D	126	HIS
1	D	128	ASN
1	D	167	ASN
1	D	170	GLN
1	D	250	ASN
1	D	255	ASN
1	D	272	ASN
1	D	286	GLN
1	A	51	ASN
1	A	128	ASN
1	A	167	ASN
1	A	170	GLN
1	A	250	ASN
1	B	98	ASN
1	B	128	ASN
1	B	170	GLN
1	B	250	ASN
1	B	255	ASN
1	B	272	ASN
1	B	286	GLN

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	287/312 (91%)	-0.30	10 (3%) 44 46	4, 18, 35, 45	9 (3%)
1	B	287/312 (91%)	-0.32	1 (0%) 94 94	6, 19, 34, 42	5 (1%)
1	C	287/312 (91%)	-0.35	5 (1%) 70 71	4, 14, 28, 36	9 (3%)
1	D	287/312 (91%)	-0.44	4 (1%) 75 77	2, 14, 26, 37	5 (1%)
All	All	1148/1248 (91%)	-0.35	20 (1%) 70 71	2, 16, 31, 45	28 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	PHE	6.1
1	A	280	ILE	3.2
1	A	128	ASN	3.0
1	A	179	THR	3.0
1	A	283	ALA	2.7
1	D	158	SER	2.7
1	C	280	ILE	2.6
1	D	280	ILE	2.5
1	C	20	PHE	2.5
1	B	281	GLN	2.4
1	D	250	ASN	2.4
1	A	250	ASN	2.3
1	A	276	GLU	2.3
1	C	250	ASN	2.3
1	A	198	TYR	2.3
1	C	281	GLN	2.3
1	A	50	ILE	2.2
1	A	171	TRP	2.2
1	D	283	ALA	2.1
1	C	179	THR	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.