



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:54 PM UTC

PDB ID : 4L8Y / pdb_00004l8y
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

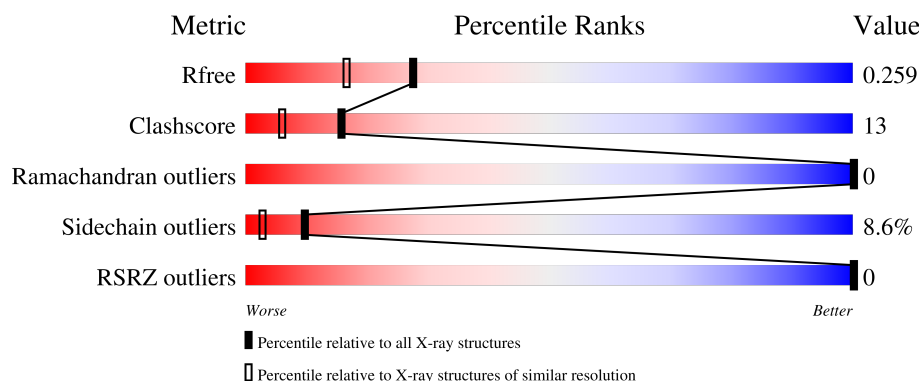
1 Overall quality at a glance

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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 $\leq 5\%$. 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	 71% 16% 8%
1	B	312	 69% 18% 8%
1	C	312	 68% 20% 8%
1	D	312	 66% 19% 5% 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

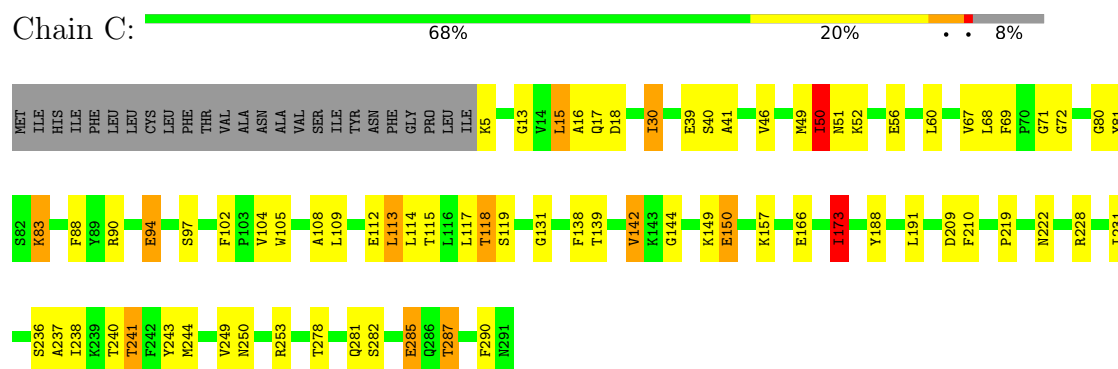
- Molecule 2 is water.

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		

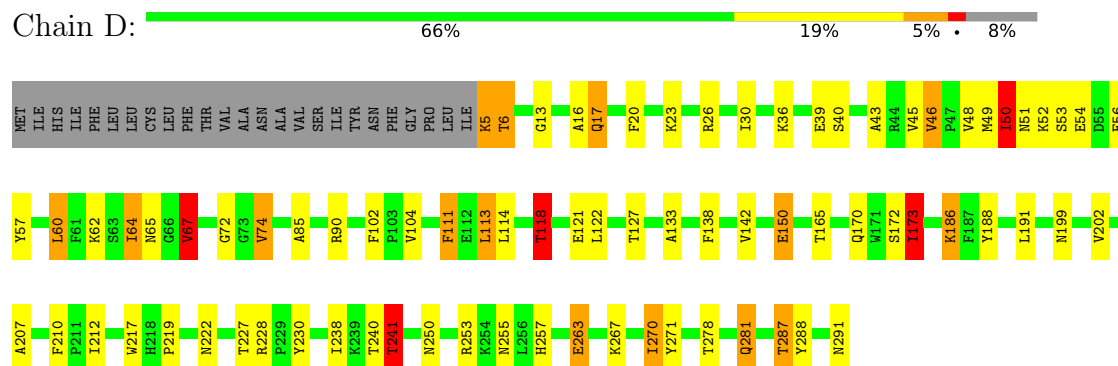
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

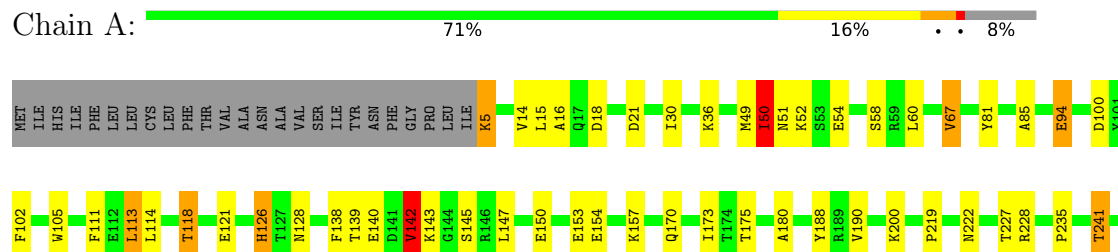
• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase

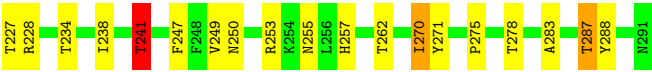
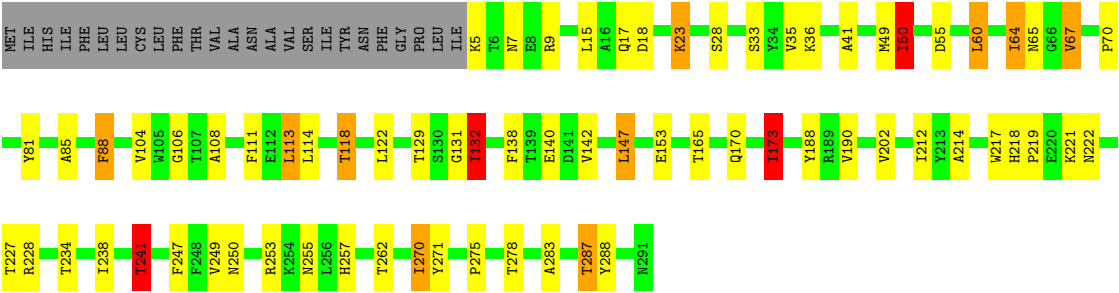


• Molecule 1: Gamma-glutamyl hydrolase





● Molecule 1: Gamma-glutamyl hydrolase



4 Data and refinement statistics

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 30.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-1.97) 99.1 (30.00-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	4376 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)	0.32 , 15.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.147 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.26	3/2373 (0.1%)	1.21	14/3220 (0.4%)
1	B	1.26	4/2373 (0.2%)	1.28	14/3220 (0.4%)
1	C	1.45	11/2373 (0.5%)	1.29	12/3220 (0.4%)
1	D	1.41	6/2373 (0.3%)	1.37	23/3220 (0.7%)
All	All	1.35	24/9492 (0.3%)	1.29	63/12880 (0.5%)

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	A	175	THR	C-O	-8.03	1.14	1.24
1	C	210	PHE	C-O	-7.62	1.16	1.24
1	D	51	ASN	N-CA	7.60	1.57	1.46
1	D	48	VAL	CA-C	-7.33	1.43	1.52
1	C	240	THR	N-CA	-6.87	1.38	1.46
1	D	133	ALA	CA-CB	-6.65	1.44	1.53
1	D	241	THR	CA-CB	6.38	1.63	1.53
1	C	104	VAL	C-O	6.12	1.30	1.24
1	C	68	LEU	N-CA	-5.97	1.38	1.46
1	C	131	GLY	C-O	-5.75	1.16	1.23
1	C	150	GLU	CD-OE1	5.71	1.36	1.25
1	B	7	ASN	N-CA	-5.67	1.39	1.46
1	A	247	PHE	C-O	5.57	1.30	1.24
1	B	67	VAL	CA-CB	5.54	1.63	1.55
1	C	236	SER	CA-C	5.53	1.60	1.52
1	B	64	ILE	CA-C	-5.51	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	ASN	C-O	-5.49	1.17	1.24
1	D	46	VAL	CA-C	5.21	1.56	1.52
1	C	237	ALA	CA-CB	5.20	1.61	1.53
1	C	51	ASN	N-CA	5.17	1.52	1.46
1	A	251	GLU	N-CA	5.17	1.52	1.46
1	D	240	THR	N-CA	-5.06	1.40	1.46
1	C	30	ILE	CA-CB	5.06	1.60	1.54
1	B	132	ILE	CG1-CD1	-5.02	1.32	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	ILE	CA-C-N	-12.43	106.05	123.20
1	D	50	ILE	C-N-CA	-12.43	106.05	123.20
1	D	50	ILE	N-CA-C	11.51	121.98	110.82
1	A	50	ILE	N-CA-C	11.08	121.76	111.45
1	C	173	ILE	CB-CA-C	-10.60	96.46	110.98
1	C	50	ILE	N-CA-C	10.55	121.37	110.72
1	C	50	ILE	CA-C-N	-10.42	101.64	121.54
1	C	50	ILE	C-N-CA	-10.42	101.64	121.54
1	B	132	ILE	CB-CA-C	-8.83	94.59	110.48
1	D	173	ILE	CB-CA-C	-8.66	99.12	110.98
1	B	190	VAL	N-CA-C	7.70	119.32	108.93
1	B	131	GLY	CA-C-N	-7.65	112.49	122.51
1	B	131	GLY	C-N-CA	-7.65	112.49	122.51
1	B	36	LYS	N-CA-C	-7.36	102.95	112.23
1	D	20	PHE	CA-C-N	-7.34	113.55	123.46
1	D	20	PHE	C-N-CA	-7.34	113.55	123.46
1	C	173	ILE	N-CA-CB	7.11	119.53	111.21
1	B	132	ILE	N-CA-C	6.65	118.74	108.44
1	C	30	ILE	CB-CA-C	-6.61	101.50	110.42
1	D	45	VAL	CA-C-N	-6.52	117.66	123.33
1	D	45	VAL	C-N-CA	-6.52	117.66	123.33
1	C	50	ILE	O-C-N	-6.37	115.27	121.83
1	B	33	SER	N-CA-C	6.26	118.91	111.33
1	B	9	ARG	CA-C-N	-6.21	113.37	119.76
1	B	9	ARG	C-N-CA	-6.21	113.37	119.76
1	B	173	ILE	CB-CA-C	-6.15	102.55	110.98
1	D	67	VAL	CG1-CB-CG2	6.12	124.27	110.80
1	A	142	VAL	CB-CA-C	-6.05	102.78	112.16
1	D	67	VAL	CB-CA-C	-6.01	99.95	110.71
1	D	6	THR	CB-CA-C	-5.98	98.99	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	SER	N-CA-C	5.87	120.17	112.89
1	C	240	THR	N-CA-C	-5.61	105.25	111.36
1	B	50	ILE	N-CA-C	5.60	117.52	111.58
1	C	243	TYR	N-CA-C	5.53	118.03	111.33
1	D	74	VAL	N-CA-CB	-5.51	102.23	111.38
1	A	157	LYS	N-CA-C	-5.50	105.37	111.36
1	D	173	ILE	N-CA-CB	5.47	117.61	111.21
1	C	150	GLU	N-CA-C	5.46	119.64	112.92
1	A	67	VAL	CG1-CB-CG2	-5.46	98.79	110.80
1	A	190	VAL	N-CA-C	5.44	116.10	109.30
1	D	17	GLN	N-CA-CB	-5.35	101.32	111.00
1	B	241	THR	CB-CA-C	5.28	120.40	110.63
1	A	228	ARG	CA-C-N	5.25	125.56	119.47
1	A	228	ARG	C-N-CA	5.25	125.56	119.47
1	A	21	ASP	CA-C-N	5.22	125.20	120.03
1	A	21	ASP	C-N-CA	5.22	125.20	120.03
1	A	145	SER	N-CA-C	5.21	117.43	110.35
1	D	74	VAL	CB-CA-C	5.18	117.29	111.59
1	A	111	PHE	N-CA-C	-5.15	105.75	111.36
1	C	97	SER	CB-CA-C	5.14	120.53	110.67
1	D	118	THR	N-CA-C	5.12	117.65	111.40
1	B	67	VAL	CB-CA-C	-5.11	101.97	111.18
1	A	36	LYS	CA-C-N	5.11	127.09	120.44
1	A	36	LYS	C-N-CA	5.11	127.09	120.44
1	D	121	GLU	N-CA-C	5.10	117.56	109.50
1	D	172	SER	CA-C-N	-5.10	116.37	122.90
1	D	172	SER	C-N-CA	-5.10	116.37	122.90
1	D	191	LEU	N-CA-C	-5.09	107.62	113.88
1	B	88	PHE	N-CA-C	5.07	117.46	111.33
1	D	241	THR	N-CA-CB	5.03	117.51	110.12
1	A	180	ALA	N-CA-C	-5.02	106.67	112.89
1	D	50	ILE	O-C-N	-5.00	115.39	121.90
1	D	67	VAL	CA-CB-CG1	5.00	118.90	110.40

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 ⓘ

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	64	0
1	B	2308	0	2229	49	0
1	C	2308	0	2229	63	0
1	D	2308	0	2229	90	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	242	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 (242) 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:HB3	1:C:83:LYS:HZ2	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:C:83:LYS:NZ	1:C:83:LYS:CB	2.37	0.85
1:B:227:THR:HG23	1:B:228:ARG:HG2	1.58	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:HE3	1:B:23:LYS:HA	1.63	0.78
1:C:83:LYS:HB3	1:C:83:LYS:HZ3	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:C:50:ILE:HD11	1:C:81:TYR:HA	1.72	0.71
1:A:280:ILE:HD12	1:A:280:ILE:H	1.53	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:D:104:VAL:HB	1:D:212:ILE:HD12	1.76	0.67
1:B:222:ASN:HB2	1:B:241:THR:HG22	1.77	0.67
1:D:230:TYR:OH	1:A:128:ASN:CG	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:NH2	1:B:238:ILE:HD13	2.14	0.63
1:B:138:PHE:CD2	1:B:142:VAL:HG11	2.32	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:217:TRP:H	1:D:217:TRP:CD1	2.16	0.62
1:C:30:ILE:HG12	1:C:290:PHE:CE1	2.34	0.62
1:B:255:ASN:ND2	1:B:257:HIS:H	1.96	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:A:5:LYS:HB3	1:A:5:LYS:HZ3	1.67	0.59
1:A:100:ASP:CG	2:A:334:HOH:O	2.45	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: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:A:250:ASN:HB3	2:A:306:HOH:O	2.03	0.58
1:B:41:ALA:HB3	1:B:249:VAL:HG21	1.85	0.57
1:B:217:TRP:H	1:B:217:TRP:CD1	2.22	0.57
1:B:255:ASN:HD21	1:B:257:HIS:CG	2.22	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:15:LEU:C	1:A:30:ILE:HD11	2.29	0.57
1:D:270:ILE:HD11	1:D:288:TYR:CZ	2.39	0.56
1:A:285:GLU:HG3	1:B:271:TYR:CE1	2.41	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:B:49:MET:HE3	1:B:49:MET:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:142:VAL:CG1	1:C:191:LEU:O	2.56	0.53
1:D:170:GLN:NE2	1:A:126:HIS:HB2	2.22	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:D:111:PHE:C	1:D:111:PHE:CD2	2.86	0.52
1:D:90:ARG:CZ	2:D:566:HOH:O	2.57	0.52
1:A:114:LEU:O	1:A:118:THR:HG23	2.09	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:65:ASN:HD22	1:D:255:ASN:ND2	2.03	0.52
1:D:127:THR:O	1:A:170:GLN:NE2	2.43	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: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:C:142:VAL:HG12	1:C:191:LEU:O	2.11	0.50
1:A:50:ILE:HD11	1:A:81:TYR:CA	2.38	0.50
1:D:230:TYR:OH	1:A:128:ASN:OD1	2.27	0.50
1:A:105:TRP:CH2	1:A:244:MET:HE3	2.46	0.50
1:C:15:LEU:HD12	1:C:69:PHE:CD2	2.47	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:A:118:THR:HG21	1:A:188:TYR:OH	2.12	0.50
1:D:64:ILE:C	1:D:64:ILE:HD13	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:HG13	2:D:539:HOH:O	2.11	0.49
1:A:285:GLU:OE1	1:A:285:GLU:CA	2.59	0.49
1:B:222:ASN:HB2	1:B:241:THR:HG21	1.93	0.49
1:D:270:ILE:HD13	1:D:270:ILE:C	2.37	0.49
1:C:228:ARG:O	1:C:231:ILE:HG12	2.13	0.49
1:A:49:MET:HB2	1:A:52:LYS:HE3	1.93	0.49
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:A:105:TRP:HH2	1:A:244:MET:HE3	1.79	0.48
1:D:49:MET:HE2	1:D:49:MET:HA	1.95	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: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:C:50:ILE:HG13	1:C:80:GLY:C	2.40	0.47
1:D:170:GLN:HG2	1:A:126:HIS:ND1	2.29	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: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:HD12	1:D:173:ILE:O	2.15	0.46
1:C:50:ILE:HG13	1:C:80:GLY:HA3	1.97	0.46
1:C:105:TRP:HH2	1:C:244:MET:HE3	1.81	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:D:278:THR:OG1	1:D:287:THR:CG2	2.63	0.46
1:B:108:ALA:O	1:B:111:PHE:HB3	2.16	0.46
1:A:94:GLU:HG2	2:A:313:HOH:O	2.16	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:A:16:ALA:HA	1:A:30:ILE:CD1	2.46	0.45
1:D:173:ILE:CD1	1:D:202:VAL:HB	2.46	0.45
1:D:170:GLN:HG2	1:A:126:HIS:NE2	2.31	0.45
1:C:49:MET:HA	1:C:49:MET:HE2	1.99	0.45
1:C:278:THR:HG21	1:C:287:THR:CG2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:TRP:CH2	1:C:244:MET:HE3	2.52	0.44
1:D:270:ILE:O	1:D:270:ILE:CD1	2.59	0.44
1:A:278:THR:OG1	1:A:287:THR:HG23	2.18	0.44
1:A:283:ALA:HB2	2:A:417:HOH:O	2.17	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:C:13:GLY:HA2	1:C:46:VAL:O	2.18	0.44
1:C:222:ASN:HB2	1:C:241:THR:HG21	1.96	0.44
1:D:281:GLN:HB2	2:D:348:HOH:O	2.18	0.44
1:A:219:PRO:O	1:A:241:THR:CG2	2.65	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:C:105:TRP:HH2	1:C:244:MET:CE	2.30	0.44
1:C:138:PHE:HB3	1:C:142:VAL:HG11	2.00	0.44
1:B:106:GLY:O	1:B:214:ALA:HA	2.18	0.44
1:D:17:GLN:OE1	1:D:72:GLY:HA3	2.19	0.43
1:D:67:VAL:HG22	1:D:102:PHE:HE2	1.82	0.43
1:D:114:LEU:O	1:D:118:THR:HG23	2.18	0.43
1:D:39:GLU:HA	1:D:43:ALA:O	2.19	0.43
1:B:85:ALA:HB3	1:B:113:LEU:HD11	2.01	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:C:71:GLY:HA2	1:C:109:LEU:HB3	2.00	0.43
1:B:218:HIS:HB3	1:B:221:LYS:HG3	2.01	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:C:40:SER:OG	1:D:40:SER:OG	2.31	0.42
1:D:186:LYS:CD	2:D:355:HOH:O	2.67	0.42
1:B:218:HIS:CG	1:B:221:LYS:HE2	2.54	0.42
1:C:250:ASN:ND2	1:C:253:ARG:HH11	2.18	0.42
1:B:67:VAL:HG11	1:B:88:PHE:CD2	2.54	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:C:90:ARG:HH11	1:C:90:ARG:HD2	1.71	0.42
1:B:173:ILE:CD1	1:B:202:VAL:HB	2.50	0.42
1:C:113:LEU:HD13	1:C:117:LEU:HD11	2.00	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:50:ILE:HD11	1:C:81:TYR:CA	2.44	0.41
1:A:16:ALA:HA	1:A:30:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:227:THR:HG22	2:D:458:HOH:O	2.20	0.41
1:B:250:ASN:ND2	1:B:253:ARG:HH11	2.19	0.41
1:B:70:PRO:HD2	1:B:81:TYR:HE1	1.86	0.41
1:B:173:ILE:HD12	1:B:202:VAL:HB	2.02	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:D:5:LYS:N	2:D:315:HOH:O	2.54	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:B:104:VAL:HB	1:B:212:ILE:HD13	2.01	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

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	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 ⓘ

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%)	226 (91%)	23 (9%)	8	2
1	B	249/271 (92%)	230 (92%)	19 (8%)	12	4
1	C	249/271 (92%)	227 (91%)	22 (9%)	9	2
1	D	249/271 (92%)	227 (91%)	22 (9%)	9	2
All	All	996/1084 (92%)	910 (91%)	86 (9%)	10	3

All (86) 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	52	LYS
1	C	56	GLU
1	C	60	LEU
1	C	83	LYS
1	C	94	GLU
1	C	113	LEU
1	C	118	THR
1	C	142	VAL
1	C	150	GLU
1	C	157	LYS
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	5	LYS
1	D	6	THR

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Mol	Chain	Res	Type
1	D	23	LYS
1	D	50	ILE
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	150	GLU
1	D	173	ILE
1	D	186	LYS
1	D	199	ASN
1	D	238	ILE
1	D	241	THR
1	D	263	GLU
1	D	270	ILE
1	D	281	GLN
1	D	287	THR
1	A	5	LYS
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	200	LYS
1	A	235	PRO
1	A	241	THR
1	A	250	ASN
1	A	258	SER
1	A	280	ILE
1	A	285	GLU

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Mol	Chain	Res	Type
1	A	287	THR
1	B	5	LYS
1	B	15	LEU
1	B	23	LYS
1	B	50	ILE
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	140	GLU
1	B	147	LEU
1	B	153	GLU
1	B	170	GLN
1	B	173	ILE
1	B	241	THR
1	B	262	THR
1	B	270	ILE
1	B	287	THR

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

Mol	Chain	Res	Type
1	C	250	ASN
1	D	51	ASN
1	D	126	HIS
1	D	128	ASN
1	D	170	GLN
1	D	250	ASN
1	D	255	ASN
1	A	27	ASN
1	A	51	ASN
1	A	128	ASN
1	A	167	ASN
1	A	170	GLN
1	A	199	ASN
1	A	250	ASN
1	A	291	ASN
1	B	98	ASN
1	B	128	ASN
1	B	170	GLN

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Mol	Chain	Res	Type
1	B	177	ASN
1	B	250	ASN
1	B	255	ASN
1	B	286	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 oligosaccharides 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	287/312 (91%)	-1.32	0 100 100	2, 17, 35, 45	9 (3%)
1	B	287/312 (91%)	-1.32	0 100 100	3, 19, 34, 42	5 (1%)
1	C	287/312 (91%)	-1.37	0 100 100	2, 14, 28, 36	9 (3%)
1	D	287/312 (91%)	-1.40	0 100 100	1, 13, 26, 37	5 (1%)
All	All	1148/1248 (91%)	-1.35	0 100 100	1, 16, 31, 45	28 (2%)

There are no RSRZ outliers to report.

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 oligosaccharides 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.