



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:43 PM UTC

PDB ID : 3AMD / pdb_00003amd
Title : Crystal structures of *Thermotoga maritima* Cel5A, apo form and tetramer/au
Authors : Wu, T.H.; Huang, C.H.; Ko, T.P.; Lai, H.L.; Ma, Y.; Cheng, Y.S.; Liu, J.R.;
Guo, R.T.
Deposited on : 2010-08-19
Resolution : 2.00 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
Xtrriage (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

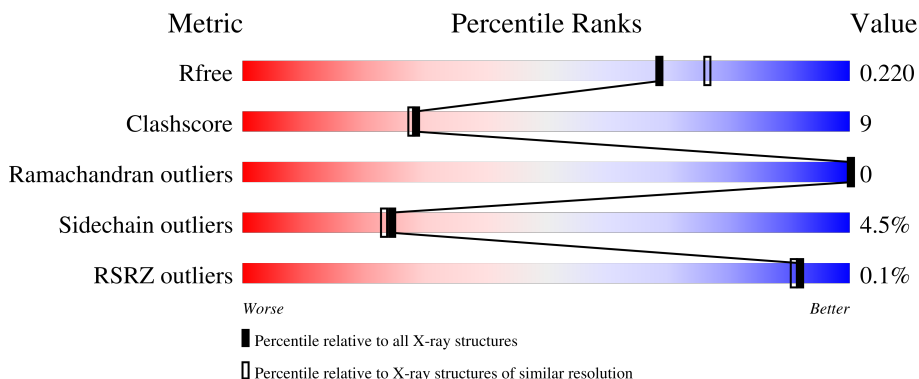
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	317	
1	B	317	
1	C	317	
1	D	317	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11201 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 Endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	Total 2610	C 1698	N 445	O 463	S 4	0	0	0
1	B	312	Total 2618	C 1703	N 446	O 464	S 5	0	0	0
1	C	309	Total 2602	C 1694	N 443	O 461	S 4	0	0	0
1	D	311	Total 2610	C 1698	N 445	O 463	S 4	0	0	0

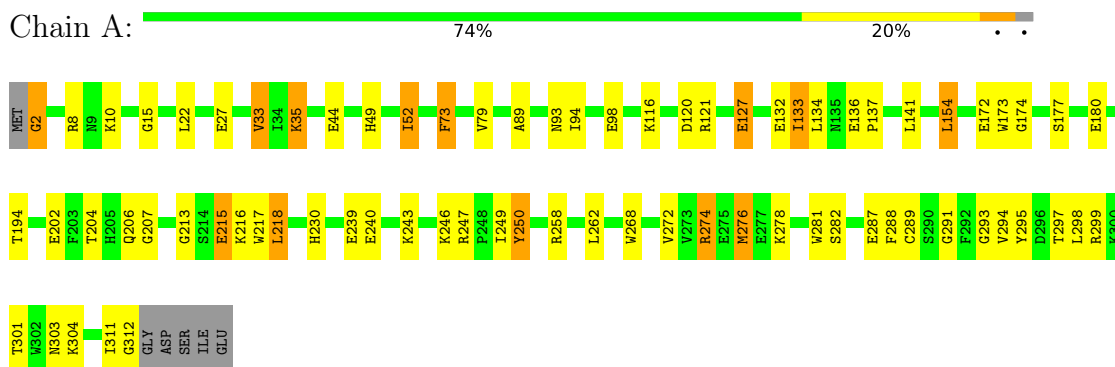
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	207	Total 207	O 207	0	0
2	B	201	Total 201	O 201	0	0
2	C	175	Total 175	O 175	0	0
2	D	178	Total 178	O 178	0	0

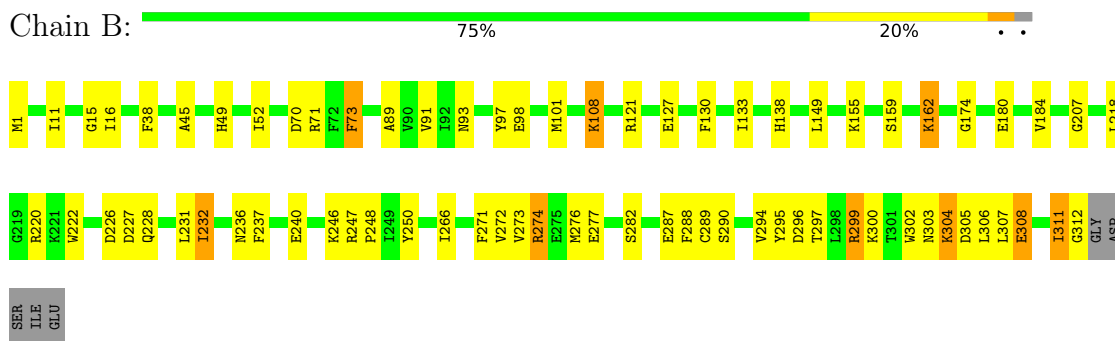
3 Residue-property plots

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.

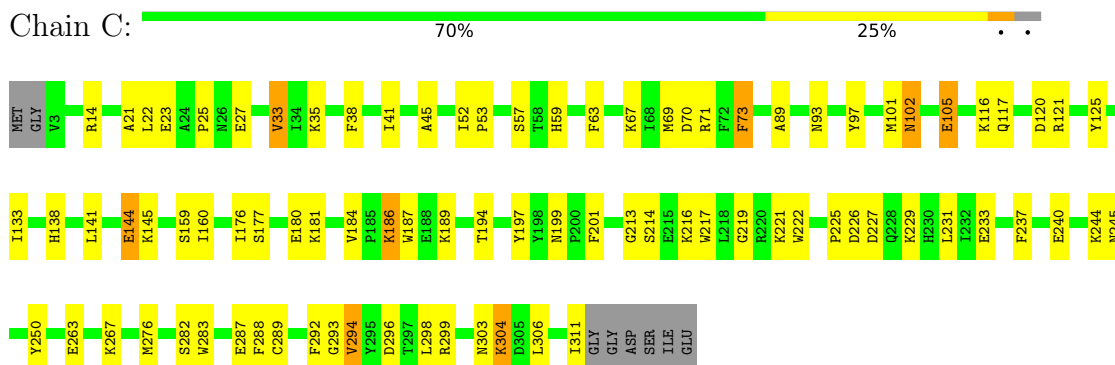
- Molecule 1: Endoglucanase



- Molecule 1: Endoglucanase

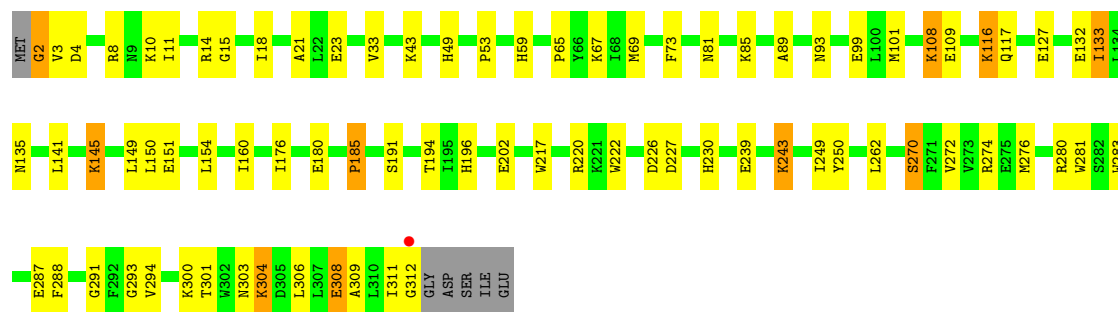


- Molecule 1: Endoglucanase



- Molecule 1: Endoglucanase

Chain D:  73% 22% ..



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.27Å 75.33Å 93.57Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-2.00) 95.8 (25.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 1.99Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.168 , 0.219 0.167 , 0.220	Depositor DCC
R_{free} test set	3797 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtrriage
Anisotropy	0.622	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11201	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.86 % 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 3.4447e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.04	2/2691 (0.1%)	1.22	21/3640 (0.6%)
1	B	1.03	1/2699 (0.0%)	1.20	15/3650 (0.4%)
1	C	1.03	4/2683 (0.1%)	1.23	26/3630 (0.7%)
1	D	1.02	5/2691 (0.2%)	1.16	17/3640 (0.5%)
All	All	1.03	12/10764 (0.1%)	1.20	79/14560 (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	A	0	1
1	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	SD-CE	7.33	1.97	1.79
1	C	21	ALA	CA-C	7.26	1.55	1.52
1	C	52	ILE	CA-CB	6.95	1.60	1.54
1	D	2	GLY	N-CA	6.33	1.55	1.45
1	A	2	GLY	N-CA	6.15	1.55	1.45
1	D	69	MET	SD-CE	6.00	1.94	1.79
1	C	69	MET	SD-CE	5.69	1.93	1.79
1	C	21	ALA	CA-CB	5.48	1.61	1.53
1	D	309	ALA	CA-CB	-5.32	1.44	1.53
1	D	101	MET	SD-CE	5.20	1.92	1.79
1	A	276	MET	SD-CE	5.20	1.92	1.79
1	D	21	ALA	CA-C	5.11	1.54	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	293	GLY	N-CA-C	10.98	124.55	111.93
1	C	133	ILE	N-CA-C	10.65	121.31	110.23
1	A	293	GLY	N-CA-C	10.03	123.47	111.93
1	B	288	PHE	N-CA-C	9.53	121.26	111.07
1	A	133	ILE	N-CA-C	9.33	119.94	110.23
1	D	288	PHE	N-CA-C	8.87	120.64	110.97
1	A	288	PHE	N-CA-C	8.82	120.58	110.97
1	B	303	ASN	N-CA-C	-8.80	95.04	108.67
1	C	293	GLY	N-CA-C	8.79	122.03	111.93
1	B	133	ILE	N-CA-C	8.01	118.56	110.23
1	B	282	SER	N-CA-C	-7.73	99.38	110.59
1	D	133	ILE	N-CA-C	7.68	118.43	110.36
1	A	52	ILE	N-CA-C	7.61	115.69	108.15
1	C	288	PHE	N-CA-C	7.46	120.13	111.02
1	D	160	ILE	N-CA-C	7.42	117.91	111.90
1	C	303	ASN	N-CA-C	-7.39	97.21	108.67
1	A	89	ALA	N-CA-C	-7.13	100.92	110.55
1	D	304	LYS	N-CA-C	7.01	118.92	111.28
1	B	89	ALA	N-CA-C	-6.63	100.70	110.52
1	D	300	LYS	N-CA-C	6.60	120.28	111.30
1	A	303	ASN	N-CA-C	-6.58	96.92	108.23
1	B	11	ILE	CB-CA-C	-6.43	103.47	112.14
1	B	311	ILE	N-CA-C	6.38	122.61	109.34
1	C	125	TYR	CA-C-N	6.34	126.31	119.78
1	C	125	TYR	C-N-CA	6.34	126.31	119.78
1	A	94	ILE	N-CA-C	-6.21	98.68	107.75
1	C	304	LYS	N-CA-C	6.20	118.55	111.11
1	A	247	ARG	CA-C-N	6.12	126.08	120.03
1	A	247	ARG	C-N-CA	6.12	126.08	120.03
1	B	290	SER	N-CA-C	6.10	114.60	108.75
1	C	33	VAL	N-CA-C	-6.07	99.61	108.11
1	C	184	VAL	CA-C-N	-6.07	113.51	119.76
1	C	184	VAL	C-N-CA	-6.07	113.51	119.76
1	C	292	PHE	N-CA-C	-6.05	105.21	112.59
1	C	294	VAL	N-CA-C	-6.03	106.86	113.43
1	B	97	TYR	N-CA-C	-5.91	101.38	109.71
1	B	304	LYS	N-CA-C	5.90	117.39	111.07
1	D	262	LEU	N-CA-C	5.86	117.34	111.07
1	B	70	ASP	N-CA-C	5.86	118.14	111.11
1	D	303	ASN	N-CA-C	-5.76	99.75	108.67
1	C	89	ALA	N-CA-C	-5.72	103.14	110.53
1	A	98	GLU	N-CA-C	5.72	117.59	111.36
1	A	136	GLU	N-CA-C	5.72	122.45	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ILE	N-CA-C	5.71	113.80	108.15
1	C	141	LEU	N-CA-C	-5.69	101.08	109.62
1	C	282	SER	N-CA-C	-5.68	102.12	110.52
1	D	33	VAL	N-CA-C	-5.64	100.22	108.11
1	C	70	ASP	N-CA-C	5.62	118.18	111.71
1	C	97	TYR	N-CA-C	-5.57	101.86	109.71
1	B	174	GLY	N-CA-C	5.56	122.75	115.36
1	D	160	ILE	CB-CA-C	-5.52	106.00	111.30
1	D	89	ALA	N-CA-C	-5.51	103.11	110.55
1	A	282	SER	N-CA-C	-5.50	102.31	110.46
1	A	289	CYS	N-CA-C	5.49	120.83	112.54
1	C	57	SER	N-CA-C	5.45	117.98	111.71
1	A	10	LYS	N-CA-C	-5.44	105.43	111.36
1	C	214	SER	N-CA-C	5.43	119.00	112.38
1	C	41	ILE	CB-CA-C	-5.42	105.04	111.97
1	B	184	VAL	N-CA-C	-5.40	101.68	108.05
1	A	262	LEU	N-CA-C	5.39	117.58	111.11
1	C	289	CYS	N-CA-C	5.35	120.62	112.54
1	D	18	ILE	N-CA-C	-5.34	98.22	109.34
1	C	102	ASN	CA-C-N	-5.33	117.42	122.37
1	C	102	ASN	C-N-CA	-5.33	117.42	122.37
1	A	304	LYS	N-CA-C	5.26	117.69	111.33
1	D	65	PRO	N-CA-C	5.25	125.75	112.10
1	A	141	LEU	N-CA-C	-5.24	99.44	108.56
1	B	289	CYS	N-CA-C	5.23	121.45	113.19
1	C	117	GLN	N-CA-C	5.23	117.06	111.36
1	D	11	ILE	CB-CA-C	-5.13	105.22	112.14
1	D	4	ASP	CA-C-N	-5.12	114.34	119.56
1	D	4	ASP	C-N-CA	-5.12	114.34	119.56
1	A	174	GLY	N-CA-C	5.09	122.37	115.30
1	A	204	THR	N-CA-C	5.08	117.71	111.82
1	C	177	SER	N-CA-C	5.07	117.54	111.71
1	C	159	SER	N-CA-C	-5.06	107.08	113.20
1	D	67	LYS	N-CA-C	5.04	117.74	110.28
1	A	177	SER	N-CA-C	5.03	117.49	111.71
1	A	33	VAL	N-CA-C	-5.01	100.44	107.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	250	TYR	Sidechain

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	2610	0	2543	47	0
1	B	2618	0	2555	47	0
1	C	2602	0	2537	46	0
1	D	2610	0	2543	48	0
2	A	207	0	0	9	0
2	B	201	0	0	3	0
2	C	175	0	0	8	0
2	D	178	0	0	11	0
All	All	11201	0	10178	182	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 9.

All (182) 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:C:304:LYS:HG2	2:C:698:HOH:O	1.60	0.99
1:B:308:GLU:OE1	1:B:312:GLY:HA3	1.63	0.99
1:B:98:GLU:HG3	2:B:354:HOH:O	1.69	0.91
1:D:133:ILE:HD11	1:D:154:LEU:HD11	1.57	0.87
1:C:33:VAL:O	1:C:35:LYS:HD2	1.77	0.85
1:D:270:SER:HB3	1:D:274:ARG:HH12	1.42	0.84
1:A:246:LYS:HD3	2:A:338:HOH:O	1.77	0.83
1:D:133:ILE:HD11	1:D:154:LEU:CD1	2.08	0.82
1:A:213:GLY:O	1:A:216:LYS:HG2	1.81	0.81
1:C:186:LYS:HD3	1:C:186:LYS:C	2.08	0.79
1:C:35:LYS:HD3	1:C:38:PHE:CZ	2.18	0.78
1:A:35:LYS:HE2	2:A:388:HOH:O	1.86	0.75
1:D:270:SER:HB3	1:D:274:ARG:NH1	2.03	0.73
1:D:99:GLU:OE1	2:D:718:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LYS:HG3	2:C:697:HOH:O	1.89	0.71
1:B:108:LYS:HD3	1:B:149:LEU:HD13	1.73	0.70
1:A:207:GLY:HA3	1:A:218:LEU:HD11	1.74	0.69
1:D:150:LEU:HD11	1:D:185:PRO:HD3	1.74	0.69
1:A:298:LEU:HA	2:C:399:HOH:O	1.93	0.69
1:B:299:ARG:CD	1:B:299:ARG:N	2.56	0.68
1:A:35:LYS:CE	2:A:388:HOH:O	2.42	0.68
1:D:304:LYS:NZ	2:D:741:HOH:O	2.27	0.66
1:A:180:GLU:HG2	2:A:420:HOH:O	1.95	0.66
1:B:299:ARG:N	1:B:299:ARG:HD2	2.10	0.66
1:C:240:GLU:OE1	2:C:403:HOH:O	2.13	0.65
1:B:266:ILE:HD13	1:B:305:ASP:HB3	1.78	0.65
1:B:308:GLU:OE2	1:C:67:LYS:HE2	1.96	0.65
1:A:240:GLU:HG3	2:A:516:HOH:O	1.97	0.64
1:A:8:ARG:NH2	1:A:127:GLU:HG3	2.13	0.64
1:A:33:VAL:O	1:A:35:LYS:HE3	1.98	0.64
1:C:180:GLU:HG3	1:C:237:PHE:HZ	1.63	0.64
1:C:186:LYS:HD3	1:C:187:TRP:N	2.13	0.63
1:C:296:ASP:OD2	1:C:299:ARG:HD3	1.98	0.63
1:B:220:ARG:HA	1:D:226:ASP:OD1	1.99	0.62
1:B:296:ASP:OD1	1:B:299:ARG:HD3	1.99	0.62
1:C:263:GLU:HG3	1:C:267:LYS:NZ	2.15	0.62
1:C:213:GLY:O	1:C:216:LYS:HG2	2.00	0.61
1:D:81:ASN:O	1:D:85:LYS:HG3	2.00	0.61
1:D:14:ARG:HG2	1:D:283:TRP:CZ2	2.36	0.61
1:A:258:ARG:HG2	1:A:291:GLY:O	2.03	0.59
1:B:299:ARG:HD3	1:B:299:ARG:H	1.68	0.58
1:B:299:ARG:CD	1:B:299:ARG:H	2.17	0.58
1:A:2:GLY:N	2:A:440:HOH:O	2.36	0.57
1:C:240:GLU:CD	2:C:403:HOH:O	2.47	0.57
1:B:228:GLN:O	1:B:232:ILE:HD12	2.05	0.56
1:A:207:GLY:CA	1:A:218:LEU:HD11	2.35	0.56
1:B:108:LYS:HD3	1:B:149:LEU:CD1	2.36	0.56
1:C:296:ASP:OD1	1:C:298:LEU:HB3	2.06	0.56
1:D:180:GLU:HG3	2:D:423:HOH:O	2.06	0.56
1:C:294:VAL:HG23	1:C:306:LEU:HB3	1.88	0.55
1:B:296:ASP:CG	1:B:299:ARG:HD3	2.32	0.55
1:B:159:SER:OG	2:B:596:HOH:O	2.18	0.55
1:A:202:GLU:HG2	1:A:217:TRP:CE2	2.41	0.55
1:B:299:ARG:HG3	1:B:299:ARG:HH11	1.71	0.55
1:B:45:ALA:O	1:B:311:ILE:HD13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:GLY:HA3	1:B:218:LEU:HD21	1.90	0.54
1:D:150:LEU:O	1:D:154:LEU:HD13	2.08	0.54
1:A:299:ARG:O	1:A:301:THR:HG23	2.08	0.54
1:B:311:ILE:O	1:B:312:GLY:C	2.50	0.53
1:C:93:ASN:C	1:C:93:ASN:OD1	2.50	0.53
1:B:38:PHE:CZ	1:B:297:THR:HG21	2.44	0.53
1:C:216:LYS:HG3	1:C:217:TRP:CD1	2.43	0.53
1:A:8:ARG:NH2	1:A:127:GLU:CG	2.72	0.53
1:A:35:LYS:NZ	2:A:382:HOH:O	2.32	0.53
1:A:73:PHE:CE2	1:A:121:ARG:HD3	2.44	0.53
1:A:33:VAL:O	1:A:35:LYS:CE	2.58	0.52
1:D:308:GLU:HA	1:D:308:GLU:OE1	2.10	0.51
1:D:222:TRP:CE2	1:D:227:ASP:HB3	2.46	0.51
1:B:273:VAL:O	1:B:277:GLU:HG2	2.11	0.51
1:A:15:GLY:HA3	1:A:49:HIS:CE1	2.45	0.51
1:D:108:LYS:HG3	1:D:109:GLU:N	2.22	0.50
1:D:291:GLY:HA3	2:D:445:HOH:O	2.11	0.50
1:A:230:HIS:HD2	2:A:417:HOH:O	1.95	0.50
1:B:15:GLY:HA3	1:B:49:HIS:CE1	2.46	0.50
1:D:135:ASN:OD1	1:D:196:HIS:HE1	1.94	0.50
1:A:298:LEU:HD23	2:C:399:HOH:O	2.12	0.49
1:D:311:ILE:O	1:D:312:GLY:C	2.56	0.49
1:C:73:PHE:CE2	1:C:121:ARG:HD3	2.48	0.48
1:D:93:ASN:OD1	1:D:93:ASN:C	2.56	0.48
1:D:230:HIS:HD2	2:D:340:HOH:O	1.96	0.48
1:A:249:ILE:HB	1:A:281:TRP:CD1	2.48	0.48
1:C:222:TRP:NE1	1:C:227:ASP:HB3	2.28	0.48
1:D:150:LEU:HD12	1:D:150:LEU:C	2.38	0.48
1:A:93:ASN:HB3	1:A:132:GLU:HB3	1.96	0.48
1:C:194:THR:HA	1:C:250:TYR:O	2.14	0.48
1:B:311:ILE:HG22	1:B:312:GLY:N	2.27	0.48
1:C:186:LYS:NZ	1:C:189:LYS:NZ	2.62	0.47
1:D:133:ILE:CD1	1:D:154:LEU:CD1	2.87	0.47
1:A:116:LYS:HD2	2:A:472:HOH:O	2.15	0.47
1:C:219:GLY:O	1:C:221:LYS:HE3	2.14	0.47
1:A:206:GLN:HB2	1:A:218:LEU:HD12	1.96	0.47
1:B:308:GLU:OE1	1:B:312:GLY:CA	2.50	0.47
1:D:116:LYS:HZ3	1:D:117:GLN:HG3	1.80	0.47
1:C:45:ALA:O	1:C:311:ILE:HD12	2.16	0.46
1:A:274:ARG:HH11	1:A:278:LYS:HG3	1.80	0.46
1:C:105:GLU:CD	1:C:145:LYS:NZ	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:GLU:O	1:D:243:LYS:HG2	2.15	0.46
1:D:59:HIS:HE1	2:D:400:HOH:O	1.98	0.46
1:C:145:LYS:NZ	2:C:418:HOH:O	2.45	0.45
1:D:141:LEU:HD12	1:D:145:LYS:HB3	1.98	0.45
1:B:71:ARG:NH2	2:B:427:HOH:O	2.49	0.45
1:A:298:LEU:HD22	1:C:181:LYS:HD3	1.97	0.45
1:D:272:VAL:HG12	1:D:276:MET:HE2	1.96	0.45
1:B:226:ASP:CG	1:D:220:ARG:HD3	2.42	0.45
1:C:101:MET:HG3	1:C:138:HIS:CE1	2.52	0.45
1:D:133:ILE:HD11	1:D:154:LEU:HD12	1.96	0.45
1:D:194:THR:HA	1:D:250:TYR:O	2.17	0.45
1:C:59:HIS:HE1	2:C:364:HOH:O	1.99	0.45
1:C:229:LYS:HE3	1:C:233:GLU:OE2	2.17	0.45
1:D:108:LYS:HD3	1:D:149:LEU:HD11	1.99	0.45
1:D:3:VAL:HG13	1:D:8:ARG:NH1	2.32	0.45
1:C:120:ASP:OD1	1:C:160:ILE:HD13	2.17	0.44
1:C:22:LEU:HD23	1:C:27:GLU:HB2	2.00	0.44
1:D:15:GLY:HA3	1:D:49:HIS:CE1	2.52	0.44
1:A:294:VAL:O	1:A:294:VAL:HG22	2.17	0.44
1:B:236:ASN:O	1:B:240:GLU:HG2	2.17	0.44
1:B:302:TRP:CG	1:B:307:LEU:HD22	2.53	0.44
1:C:222:TRP:CE2	1:C:227:ASP:HB3	2.53	0.44
1:A:215:GLU:H	1:A:215:GLU:HG2	1.47	0.44
1:A:239:GLU:O	1:A:243:LYS:HG2	2.18	0.44
1:C:197:TYR:CZ	1:C:199:ASN:HB2	2.53	0.44
1:D:154:LEU:HD22	1:D:185:PRO:HG2	1.99	0.44
1:C:23:GLU:HB3	1:C:53:PRO:HB2	2.00	0.44
1:B:93:ASN:OD1	1:B:93:ASN:C	2.60	0.44
1:D:43:LYS:HE2	2:D:747:HOH:O	2.17	0.44
1:A:216:LYS:NZ	1:A:217:TRP:HE1	2.16	0.43
1:A:272:VAL:O	1:A:276:MET:HG3	2.18	0.43
1:B:101:MET:HG3	1:B:138:HIS:CE1	2.53	0.43
1:B:73:PHE:CE2	1:B:121:ARG:HD3	2.53	0.43
1:B:91:VAL:HG22	1:B:130:PHE:HB2	1.99	0.43
1:B:231:LEU:HD11	1:B:272:VAL:HG22	2.01	0.43
1:C:14:ARG:HG2	1:C:283:TRP:CZ2	2.54	0.43
1:A:133:ILE:HD11	1:A:154:LEU:HD13	2.01	0.43
1:C:105:GLU:OE1	1:C:145:LYS:NZ	2.50	0.42
1:B:180:GLU:CG	1:B:237:PHE:HZ	2.32	0.42
1:C:73:PHE:CD2	1:C:121:ARG:HD3	2.54	0.42
1:C:144:GLU:CD	1:C:144:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:LYS:HD2	1:C:245:ASN:ND2	2.34	0.42
1:D:127:GLU:HG3	2:D:415:HOH:O	2.18	0.42
1:A:52:ILE:HD13	1:A:79:VAL:HG12	2.01	0.42
1:B:306:LEU:HA	1:B:306:LEU:HD23	1.80	0.42
1:D:2:GLY:N	2:D:490:HOH:O	2.52	0.42
1:B:162:LYS:HE2	1:B:162:LYS:HB2	1.86	0.42
1:B:274:ARG:HA	1:B:274:ARG:HD3	1.64	0.42
1:A:93:ASN:OD1	1:A:93:ASN:C	2.62	0.42
1:B:273:VAL:HA	1:B:276:MET:HE2	2.01	0.42
1:D:308:GLU:HG2	2:D:740:HOH:O	2.19	0.42
1:B:180:GLU:CD	1:B:237:PHE:HZ	2.28	0.42
1:C:276:MET:HE3	1:C:283:TRP:CD1	2.55	0.42
1:C:35:LYS:HD2	1:C:35:LYS:N	2.35	0.42
1:D:311:ILE:O	1:D:312:GLY:O	2.38	0.42
1:A:268:TRP:O	1:A:272:VAL:HG23	2.20	0.42
1:B:232:ILE:HD11	1:B:271:PHE:HZ	1.84	0.41
1:B:295:TYR:CZ	1:B:300:LYS:HA	2.55	0.41
1:D:93:ASN:HB3	1:D:132:GLU:HB3	2.02	0.41
1:D:249:ILE:HB	1:D:281:TRP:CD1	2.55	0.41
1:D:176:ILE:HG12	2:D:710:HOH:O	2.20	0.41
1:D:294:VAL:HG12	1:D:306:LEU:HB3	2.01	0.41
1:D:294:VAL:HG12	1:D:306:LEU:HD13	2.02	0.41
1:A:172:GLU:O	1:A:173:TRP:HB2	2.21	0.41
1:A:22:LEU:HD23	1:A:27:GLU:HB2	2.03	0.41
1:C:306:LEU:HA	1:C:306:LEU:HD23	1.76	0.41
1:A:194:THR:HA	1:A:250:TYR:O	2.21	0.41
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.85	0.41
1:A:311:ILE:O	1:A:312:GLY:C	2.63	0.41
1:B:274:ARG:HG2	1:C:63:PHE:CE2	2.56	0.41
1:C:33:VAL:H	1:C:35:LYS:NZ	2.18	0.41
1:C:176:ILE:HG21	1:C:176:ILE:HD13	1.78	0.41
1:D:306:LEU:HD23	1:D:306:LEU:HA	1.86	0.41
1:A:116:LYS:HE2	1:A:116:LYS:HB3	1.91	0.41
1:A:274:ARG:NH1	1:A:278:LYS:HG3	2.37	0.40
1:B:220:ARG:HG3	1:D:226:ASP:CG	2.45	0.40
1:A:295:TYR:CE2	1:A:297:THR:HA	2.56	0.40
1:D:202:GLU:HA	1:D:217:TRP:CE3	2.56	0.40
1:A:134:LEU:HD23	1:A:137:PRO:HG3	2.03	0.40
1:B:222:TRP:NE1	1:B:227:ASP:HB3	2.37	0.40
1:B:246:LYS:HD3	1:B:246:LYS:HA	1.83	0.40
1:C:35:LYS:HD2	1:C:35:LYS:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PHE:CZ	1:A:121:ARG:HD3	2.56	0.40
1:B:247:ARG:HA	1:B:248:PRO:HD3	1.98	0.40
1:B:294:VAL:HG22	1:B:294:VAL:O	2.21	0.40
1:D:23:GLU:HB3	1:D:53:PRO:HB2	2.03	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	309/317 (98%)	301 (97%)	8 (3%)	0	100	100
1	B	310/317 (98%)	299 (96%)	11 (4%)	0	100	100
1	C	307/317 (97%)	295 (96%)	12 (4%)	0	100	100
1	D	309/317 (98%)	302 (98%)	7 (2%)	0	100	100
All	All	1235/1268 (97%)	1197 (97%)	38 (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	272/277 (98%)	262 (96%)	10 (4%)	30	30
1	B	273/277 (99%)	261 (96%)	12 (4%)	25	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	272/277 (98%)	259 (95%)	13 (5%)	23	21
1	D	272/277 (98%)	258 (95%)	14 (5%)	21	19
All	All	1089/1108 (98%)	1040 (96%)	49 (4%)	24	23

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	44	GLU
1	A	73	PHE
1	A	120	ASP
1	A	127	GLU
1	A	154	LEU
1	A	215	GLU
1	A	218	LEU
1	A	274	ARG
1	A	287	GLU
1	B	16	ILE
1	B	73	PHE
1	B	108	LYS
1	B	127	GLU
1	B	155	LYS
1	B	162	LYS
1	B	232	ILE
1	B	274	ARG
1	B	287	GLU
1	B	299	ARG
1	B	304	LYS
1	B	308	GLU
1	C	25	PRO
1	C	71	ARG
1	C	73	PHE
1	C	102	ASN
1	C	105	GLU
1	C	116	LYS
1	C	144	GLU
1	C	186	LYS
1	C	201	PHE
1	C	225	PRO
1	C	226	ASP
1	C	231	LEU

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Mol	Chain	Res	Type
1	C	287	GLU
1	D	10	LYS
1	D	73	PHE
1	D	108	LYS
1	D	116	LYS
1	D	145	LYS
1	D	151	GLU
1	D	185	PRO
1	D	191	SER
1	D	243	LYS
1	D	270	SER
1	D	280	ARG
1	D	287	GLU
1	D	301	THR
1	D	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	205	HIS
1	A	230	HIS
1	B	81	ASN
1	B	138	HIS
1	B	245	ASN
1	C	59	HIS
1	D	20	ASN
1	D	59	HIS
1	D	230	HIS

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	311/317 (98%)	-0.62	0 100 100	9, 17, 29, 39	0
1	B	312/317 (98%)	-0.62	0 100 100	10, 17, 29, 40	0
1	C	309/317 (97%)	-0.54	0 100 100	12, 19, 29, 42	0
1	D	311/317 (98%)	-0.55	1 (0%) 90 89	10, 19, 32, 38	0
All	All	1243/1268 (98%)	-0.58	1 (0%) 92 91	9, 18, 29, 42	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	GLY	2.3

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.