



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2021 – 10:08 AM JST

PDB ID : 6M3U
Title : Crystal structure of the mouse endonuclease EndoG(H138A/C100A), space group C2
Authors : Park, K.H.; Woo, E.J.
Deposited on : 2020-03-04
Resolution : 2.32 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

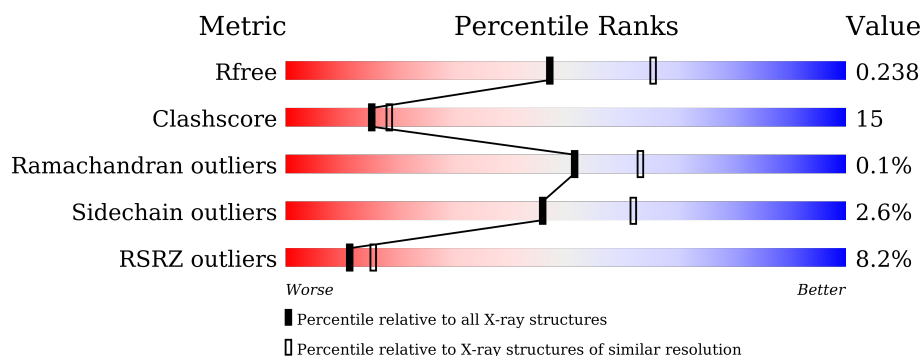
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	249	
1	B	249	
1	C	249	
1	D	249	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7636 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 Endonuclease G, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1834	1158	338	335	3			
1	B	232	Total	C	N	O	S	0	0	0
			1842	1162	339	338	3			
1	C	230	Total	C	N	O	S	1	0	0
			1831	1156	337	335	3			
1	D	232	Total	C	N	O	S	0	0	0
			1843	1163	339	338	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	engineered mutation	UNP O08600
A	138	ALA	HIS	engineered mutation	UNP O08600
B	110	ALA	CYS	engineered mutation	UNP O08600
B	138	ALA	HIS	engineered mutation	UNP O08600
C	110	ALA	CYS	engineered mutation	UNP O08600
C	138	ALA	HIS	engineered mutation	UNP O08600
D	110	ALA	CYS	engineered mutation	UNP O08600
D	138	ALA	HIS	engineered mutation	UNP O08600

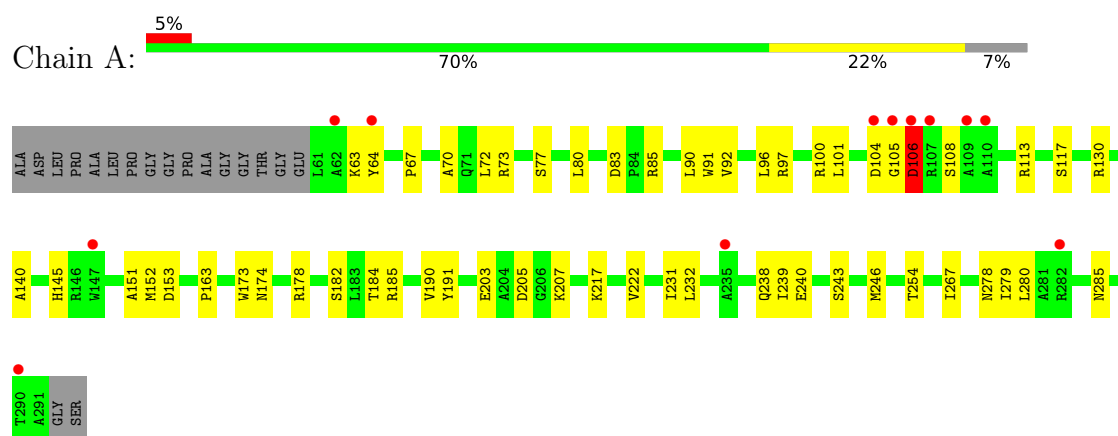
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total	O	0	0
			87	87		
2	B	54	Total	O	0	0
			54	54		
2	C	74	Total	O	0	0
			74	74		
2	D	71	Total	O	0	0
			71	71		

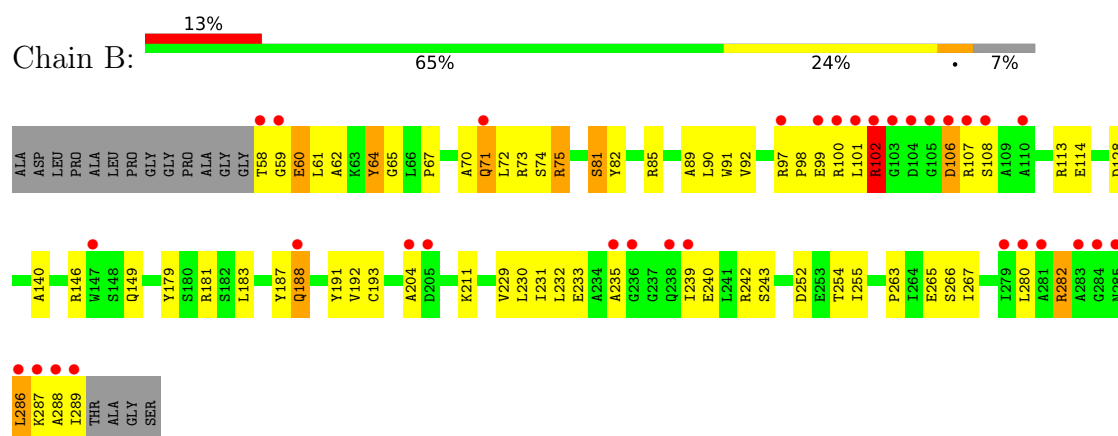
3 Residue-property plots [i](#)

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.

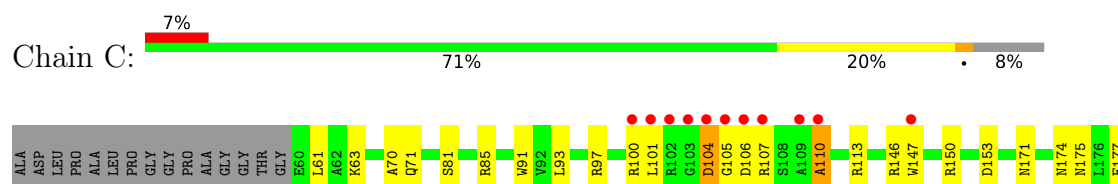
- Molecule 1: Endonuclease G, mitochondrial

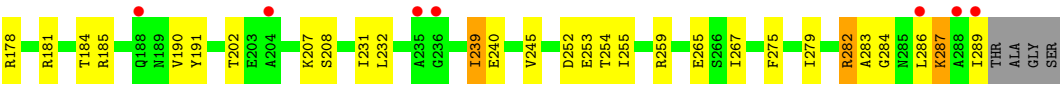


- Molecule 1: Endonuclease G, mitochondrial

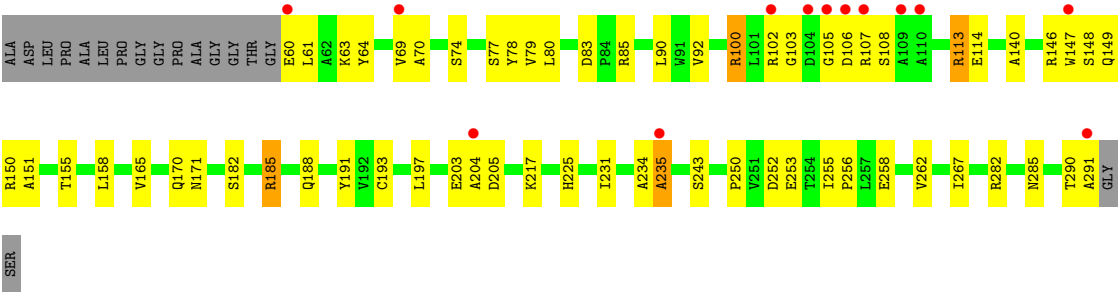


- Molecule 1: Endonuclease G, mitochondrial





● Molecule 1: Endonuclease G, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	252.41Å 81.34Å 54.68Å 90.00° 102.17° 90.00°	Depositor
Resolution (Å)	42.19 – 2.32 42.19 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.6 (42.19-2.32) 97.6 (42.19-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.201 , 0.237 0.201 , 0.238	Depositor DCC
R_{free} test set	2297 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7636	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.33	0/1878	0.64	4/2553 (0.2%)
1	B	0.38	0/1886	0.68	5/2563 (0.2%)
1	C	0.32	0/1875	0.59	2/2548 (0.1%)
1	D	0.44	1/1887 (0.1%)	0.69	7/2565 (0.3%)
All	All	0.37	1/7526 (0.0%)	0.65	18/10229 (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	A	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	185	ARG	CZ-NH2	5.33	1.40	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	ALA	C-N-CA	11.67	150.88	121.70
1	A	280	LEU	CB-CA-C	-9.53	92.09	110.20
1	D	185	ARG	CG-CD-NE	-9.28	92.31	111.80
1	D	235	ALA	CB-CA-C	-9.12	96.42	110.10
1	D	185	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	D	185	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	64	TYR	CB-CA-C	7.35	125.10	110.40
1	D	185	ARG	NH1-CZ-NH2	7.21	127.33	119.40
1	C	110	ALA	C-N-CA	-6.52	105.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	185	ARG	CA-CB-CG	-5.78	100.69	113.40
1	B	60	GLU	O-C-N	5.47	131.45	122.70
1	B	102	ARG	CB-CA-C	5.45	121.30	110.40
1	A	105	GLY	C-N-CA	5.35	135.08	121.70
1	D	171	ASN	O-C-N	-5.31	114.20	122.70
1	B	59	GLY	C-N-CA	-5.29	108.48	121.70
1	A	279	ILE	O-C-N	5.19	131.00	122.70
1	A	279	ILE	C-N-CA	5.16	134.60	121.70
1	C	287	LYS	O-C-N	5.07	130.82	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ASP	Mainchain
1	C	104	ASP	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	1834	0	1805	40	2
1	B	1842	0	1806	71	30
1	C	1831	0	1799	60	15
1	D	1843	0	1811	66	30
2	A	87	0	0	8	0
2	B	54	0	0	11	0
2	C	74	0	0	8	0
2	D	71	0	0	21	0
All	All	7636	0	7221	217	47

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 15.

All (217) 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:B:89:ALA:HA	2:B:301:HOH:O	1.20	1.38
1:C:184:THR:CB	2:C:301:HOH:O	1.86	1.19
1:C:184:THR:HB	2:C:301:HOH:O	1.41	1.18
1:D:103:GLY:O	1:D:106:ASP:OD1	1.67	1.12
1:A:70:ALA:HB2	1:B:70:ALA:HB2	1.23	1.09
1:B:101:LEU:HD21	1:B:181:ARG:HD2	1.27	1.08
1:B:263:PRO:HA	1:B:289:ILE:HG23	1.36	1.06
1:B:71:GLN:HA	1:B:71:GLN:OE1	1.52	1.06
1:D:291:ALA:N	2:D:301:HOH:O	1.88	1.05
1:B:211:LYS:NZ	2:B:302:HOH:O	1.89	1.04
1:D:291:ALA:HB2	2:D:301:HOH:O	1.57	1.01
1:A:130:ARG:NH2	2:A:301:HOH:O	1.81	1.01
1:B:90:LEU:N	2:B:301:HOH:O	1.93	0.99
1:A:130:ARG:NH1	2:A:301:HOH:O	1.94	0.99
1:B:89:ALA:CA	2:B:301:HOH:O	1.87	0.99
1:D:204:ALA:HB3	2:D:310:HOH:O	1.64	0.98
1:D:69:VAL:HG12	1:D:70:ALA:H	1.29	0.96
1:D:147:TRP:NE1	2:D:303:HOH:O	1.92	0.94
1:D:291:ALA:CB	2:D:301:HOH:O	2.14	0.94
1:C:207:LYS:NZ	2:C:302:HOH:O	1.98	0.94
1:C:104:ASP:CG	1:C:107:ARG:HB2	1.89	0.93
1:B:81:SER:O	2:B:301:HOH:O	1.86	0.92
1:D:60:GLU:HG3	1:D:63:LYS:HB2	1.52	0.92
1:B:211:LYS:NZ	2:B:303:HOH:O	2.03	0.91
1:B:188:GLN:OE1	1:B:235:ALA:HA	1.72	0.90
1:D:291:ALA:O	2:D:302:HOH:O	1.88	0.88
1:A:104:ASP:HB2	1:A:106:ASP:OD1	1.75	0.86
1:B:101:LEU:CD2	1:B:181:ARG:HD2	2.08	0.84
1:C:184:THR:OG1	2:C:301:HOH:O	1.86	0.83
1:D:290:THR:C	2:D:302:HOH:O	2.17	0.81
1:A:63:LYS:O	1:B:282:ARG:HD3	1.80	0.80
1:A:285:ASN:O	2:A:303:HOH:O	2.01	0.78
1:D:203:GLU:OE1	2:D:305:HOH:O	2.00	0.78
1:D:155:THR:OG1	2:D:306:HOH:O	2.02	0.77
1:D:285:ASN:O	2:D:307:HOH:O	2.02	0.76
1:B:233:GLU:HA	1:B:239:ILE:HD13	1.67	0.76
1:C:97:ARG:HD3	1:C:100:ARG:HH12	1.50	0.75
1:D:114:GLU:OE2	2:D:308:HOH:O	2.05	0.74
1:C:104:ASP:OD2	1:C:107:ARG:HB2	1.86	0.74
1:C:97:ARG:HD3	1:C:100:ARG:NH1	2.04	0.73
1:C:71:GLN:HA	1:C:71:GLN:OE1	1.88	0.73
1:D:147:TRP:CE2	2:D:303:HOH:O	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLU:OE1	2:C:303:HOH:O	2.07	0.72
1:C:113:ARG:HH11	1:C:113:ARG:HG3	1.54	0.72
1:C:240:GLU:CD	1:C:289:ILE:HD11	2.10	0.71
1:C:239:ILE:HD12	1:C:283:ALA:HB1	1.71	0.71
1:D:205:ASP:N	2:D:310:HOH:O	2.22	0.71
1:B:71:GLN:OE1	1:B:71:GLN:CA	2.30	0.70
1:C:175:ASN:OD1	2:C:304:HOH:O	2.09	0.70
1:D:60:GLU:CG	1:D:63:LYS:HB2	2.22	0.70
1:C:104:ASP:OD2	1:C:146:ARG:HG2	1.92	0.69
1:B:102:ARG:NH2	1:B:106:ASP:H	1.78	0.69
1:C:286:LEU:O	1:C:287:LYS:HG2	1.93	0.68
1:B:192:VAL:HG13	1:B:230:LEU:HD23	1.74	0.68
1:C:110:ALA:HB2	1:C:153:ASP:OD1	1.94	0.68
1:C:190:VAL:HG13	1:C:232:LEU:HD23	1.75	0.68
1:D:147:TRP:CZ2	2:D:303:HOH:O	2.47	0.68
1:C:104:ASP:C	1:C:106:ASP:H	1.95	0.67
1:B:263:PRO:HA	1:B:289:ILE:CG2	2.20	0.67
1:D:188:GLN:OE1	1:D:235:ALA:HB2	1.94	0.67
1:B:82:TYR:HA	2:B:301:HOH:O	1.94	0.67
1:B:265:GLU:OE2	2:B:305:HOH:O	2.11	0.67
1:B:108:SER:HB3	1:B:149:GLN:OE1	1.95	0.67
1:B:113:ARG:HE	1:B:114:GLU:HG2	1.59	0.67
1:D:69:VAL:HG12	1:D:70:ALA:N	2.08	0.67
1:D:100:ARG:HA	1:D:147:TRP:HB3	1.76	0.66
1:D:103:GLY:O	1:D:106:ASP:CG	2.33	0.66
1:B:204:ALA:N	2:B:304:HOH:O	2.06	0.66
1:C:100:ARG:HA	1:C:147:TRP:HB3	1.77	0.66
1:B:243:SER:HB2	1:B:267:ILE:HD12	1.79	0.65
1:C:202:THR:HG22	1:C:208:SER:OG	1.96	0.65
1:C:177:GLU:OE2	2:C:305:HOH:O	2.14	0.65
1:D:291:ALA:CA	2:D:301:HOH:O	2.28	0.65
1:B:97:ARG:O	1:B:100:ARG:HB2	1.96	0.64
1:B:102:ARG:HG3	1:B:146:ARG:C	2.17	0.63
1:C:113:ARG:HG3	1:C:113:ARG:NH1	2.12	0.63
1:D:290:THR:O	2:D:302:HOH:O	2.15	0.63
1:A:191:TYR:HB2	1:A:231:ILE:HB	1.81	0.62
1:B:240:GLU:HG2	1:B:287:LYS:HZ2	1.65	0.62
1:B:204:ALA:CB	2:B:304:HOH:O	2.47	0.62
1:A:207:LYS:NZ	2:A:302:HOH:O	1.81	0.62
1:B:263:PRO:CA	1:B:289:ILE:HG23	2.23	0.62
1:A:205:ASP:OD2	2:A:304:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ARG:HH22	1:D:85:ARG:HH22	1.49	0.61
1:C:174:ASN:O	1:C:178:ARG:HG3	2.01	0.61
1:A:108:SER:O	1:A:108:SER:OG	2.18	0.60
1:B:280:LEU:HD21	1:B:286:LEU:HD22	1.84	0.60
1:A:70:ALA:HB2	1:B:70:ALA:CB	2.16	0.59
1:D:105:GLY:O	1:D:107:ARG:CD	2.51	0.59
1:D:258:GLU:H	1:D:258:GLU:CD	2.06	0.59
1:B:101:LEU:HD21	1:B:181:ARG:CD	2.18	0.58
1:A:278:ASN:ND2	1:B:65:GLY:HA3	2.18	0.58
1:D:105:GLY:O	1:D:107:ARG:HD3	2.03	0.58
1:D:188:GLN:HB2	1:D:235:ALA:HB2	1.85	0.58
1:C:207:LYS:HB3	2:D:346:HOH:O	2.04	0.58
1:C:104:ASP:CG	1:C:107:ARG:CB	2.69	0.58
1:A:173:TRP:HE3	1:A:246:MET:HE3	1.69	0.57
1:A:85:ARG:HH22	1:B:85:ARG:HH22	1.52	0.57
1:A:130:ARG:CZ	2:A:301:HOH:O	2.13	0.57
1:D:243:SER:HB3	1:D:267:ILE:HD12	1.86	0.57
1:B:240:GLU:HG2	1:B:287:LYS:NZ	2.20	0.56
1:C:150:ARG:HG3	1:C:150:ARG:NH1	2.21	0.56
1:C:150:ARG:HG3	1:C:150:ARG:HH11	1.69	0.56
1:C:240:GLU:OE2	1:C:289:ILE:HD11	2.06	0.56
1:C:275:PHE:O	1:C:279:ILE:HG12	2.04	0.56
1:B:233:GLU:HA	1:B:239:ILE:CD1	2.36	0.56
1:D:234:ALA:O	1:D:235:ALA:HB3	2.06	0.56
1:B:62:ALA:O	1:B:64:TYR:O	2.24	0.56
1:B:204:ALA:HB2	2:B:304:HOH:O	2.06	0.55
1:C:191:TYR:HB2	1:C:231:ILE:HB	1.89	0.55
1:B:113:ARG:NE	1:B:114:GLU:H	2.05	0.54
1:C:81:SER:HB2	1:C:91:TRP:CE2	2.43	0.54
1:C:190:VAL:HG13	1:C:232:LEU:CD2	2.37	0.54
1:D:204:ALA:CA	2:D:310:HOH:O	2.56	0.54
1:D:83:ASP:HB2	1:D:90:LEU:HG	1.89	0.54
1:A:203:GLU:OE2	2:A:305:HOH:O	2.18	0.53
1:B:102:ARG:HD3	1:B:146:ARG:HB3	1.91	0.53
1:C:71:GLN:OE1	1:C:71:GLN:CA	2.56	0.53
1:B:74:SER:C	1:B:75:ARG:HD2	2.29	0.53
1:B:280:LEU:HD21	1:B:286:LEU:CD2	2.38	0.53
1:C:286:LEU:HG	1:C:287:LYS:H	1.74	0.53
1:C:104:ASP:C	1:C:106:ASP:N	2.62	0.52
1:C:252:ASP:HB3	1:C:255:ILE:HD12	1.90	0.52
1:A:64:TYR:OH	1:B:239:ILE:HD11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:H	1:A:238:GLN:CD	2.13	0.52
1:D:252:ASP:HB3	1:D:255:ILE:HG13	1.92	0.52
1:B:75:ARG:HD2	1:B:75:ARG:N	2.25	0.51
1:C:252:ASP:HB3	1:C:255:ILE:CD1	2.39	0.51
1:A:239:ILE:HD11	1:B:64:TYR:OH	2.10	0.51
1:A:243:SER:HB3	1:A:267:ILE:HD12	1.92	0.51
1:B:243:SER:HB2	1:B:267:ILE:CD1	2.40	0.51
1:C:239:ILE:HD11	1:C:286:LEU:HD12	1.93	0.51
1:D:92:VAL:O	1:D:193:CYS:HA	2.11	0.51
1:D:158:LEU:HB2	2:D:321:HOH:O	2.10	0.51
1:A:83:ASP:HB2	1:A:90:LEU:HG	1.93	0.50
1:D:63:LYS:HD3	1:D:64:TYR:CE1	2.46	0.50
1:B:92:VAL:HG11	1:B:140:ALA:HB2	1.92	0.50
1:B:128:ASP:O	1:D:285:ASN:ND2	2.45	0.50
1:D:191:TYR:HB2	1:D:231:ILE:HB	1.94	0.49
1:D:256:PRO:HB3	1:D:258:GLU:OE2	2.12	0.49
1:A:96:LEU:HB2	1:A:190:VAL:HB	1.93	0.49
1:B:102:ARG:CD	1:B:146:ARG:HB3	2.42	0.49
1:B:60:GLU:CD	1:B:61:LEU:H	2.16	0.48
1:B:179:TYR:CE2	1:B:183:LEU:HD11	2.48	0.48
1:B:187:TYR:CE2	1:B:232:LEU:HD13	2.49	0.48
1:C:282:ARG:O	1:C:284:GLY:N	2.47	0.48
1:C:61:LEU:HD21	1:D:79:VAL:HG12	1.95	0.48
1:A:63:LYS:NZ	1:A:64:TYR:CZ	2.82	0.47
1:B:73:ARG:HH11	1:B:73:ARG:HG2	1.79	0.47
1:A:113:ARG:NH2	1:A:153:ASP:O	2.46	0.47
1:B:92:VAL:O	1:B:193:CYS:HA	2.14	0.47
1:A:77:SER:HB3	1:A:151:ALA:HB1	1.96	0.47
1:D:114:GLU:CD	2:D:308:HOH:O	2.51	0.47
1:C:70:ALA:O	1:C:71:GLN:OE1	2.33	0.47
1:D:105:GLY:O	1:D:106:ASP:C	2.53	0.47
1:D:69:VAL:CG1	1:D:70:ALA:H	2.11	0.46
1:D:92:VAL:HG11	1:D:140:ALA:HB2	1.96	0.46
1:D:107:ARG:CD	1:D:146:ARG:HD3	2.45	0.46
1:C:255:ILE:HG23	1:C:259:ARG:HD3	1.97	0.46
1:D:243:SER:HB2	1:D:262:VAL:O	2.16	0.46
1:C:171:ASN:HB3	1:C:253:GLU:HB3	1.97	0.46
1:B:102:ARG:CG	1:B:146:ARG:O	2.64	0.46
1:C:150:ARG:HH11	1:C:150:ARG:CG	2.29	0.46
1:A:73:ARG:NH2	1:A:117:SER:O	2.48	0.45
1:A:232:LEU:HB2	1:A:240:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ALA:HB2	1:D:64:TYR:HE2	1.81	0.45
1:D:77:SER:HB3	1:D:151:ALA:HB1	1.98	0.45
1:D:105:GLY:O	1:D:107:ARG:HG3	2.16	0.45
1:B:102:ARG:HG3	1:B:146:ARG:O	2.16	0.45
1:C:240:GLU:CG	1:C:289:ILE:HD11	2.47	0.45
1:D:188:GLN:CG	1:D:235:ALA:HB2	2.47	0.45
1:A:163:PRO:HB2	1:A:222:VAL:HG22	1.98	0.44
1:B:191:TYR:HB2	1:B:231:ILE:HB	1.99	0.44
1:A:91:TRP:CD2	1:B:67:PRO:HG2	2.52	0.44
1:A:92:VAL:HG11	1:A:140:ALA:HB2	1.99	0.44
1:C:101:LEU:HD13	1:C:181:ARG:HB3	1.98	0.44
1:D:217:LYS:HB3	1:D:217:LYS:HE2	1.85	0.44
1:D:165:VAL:HG11	1:D:250:PRO:HD3	2.00	0.44
1:A:174:ASN:O	1:A:178:ARG:HG3	2.17	0.44
1:B:113:ARG:HE	1:B:114:GLU:H	1.65	0.44
1:A:145:HIS:O	1:A:152:MET:HG3	2.18	0.44
1:A:178:ARG:NH2	2:A:313:HOH:O	2.51	0.43
1:D:113:ARG:O	1:D:158:LEU:HG	2.18	0.43
1:B:263:PRO:O	1:B:266:SER:HB2	2.18	0.43
1:A:67:PRO:HD2	1:B:91:TRP:CE2	2.53	0.43
1:A:97:ARG:NH1	1:B:58:THR:N	2.66	0.43
1:B:229:VAL:HG22	1:B:243:SER:HB3	2.01	0.43
1:C:104:ASP:HA	1:C:106:ASP:H	1.83	0.43
1:D:197:LEU:HB2	1:D:225:HIS:HB2	2.00	0.43
1:C:85:ARG:NH2	1:D:85:ARG:HH22	2.16	0.43
1:B:179:TYR:OH	1:B:242:ARG:NH1	2.52	0.42
1:C:240:GLU:HG3	1:C:287:LYS:O	2.19	0.42
1:A:72:LEU:HD23	1:A:80:LEU:O	2.19	0.42
1:B:64:TYR:CD1	1:B:64:TYR:N	2.87	0.42
1:A:278:ASN:CB	1:B:65:GLY:HA3	2.49	0.42
1:B:72:LEU:HD23	1:B:81:SER:HB2	1.99	0.42
1:C:70:ALA:HB2	1:D:70:ALA:HB2	2.00	0.42
1:D:204:ALA:N	2:D:310:HOH:O	2.52	0.42
1:D:78:TYR:CE1	1:D:80:LEU:HD23	2.54	0.42
1:B:192:VAL:HG13	1:B:230:LEU:CD2	2.46	0.42
1:A:101:LEU:HD12	1:A:184:THR:HG21	2.02	0.42
1:B:102:ARG:HD2	1:B:146:ARG:O	2.19	0.41
1:C:245:VAL:HG23	1:C:267:ILE:HD11	2.02	0.41
1:D:60:GLU:HG3	1:D:60:GLU:O	2.20	0.41
1:C:104:ASP:CA	1:C:106:ASP:H	2.32	0.41
1:D:253:GLU:H	1:D:253:GLU:HG2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ASP:CG	1:C:146:ARG:HG2	2.40	0.41
1:C:106:ASP:HB2	1:C:146:ARG:O	2.21	0.41
1:D:108:SER:HB2	1:D:149:GLN:OE1	2.21	0.41
1:A:97:ARG:HB2	1:A:100:ARG:HD3	2.03	0.40
1:C:93:LEU:HG	1:D:61:LEU:CD2	2.51	0.40
1:B:97:ARG:HB3	1:B:98:PRO:HD2	2.02	0.40
1:C:63:LYS:HE3	1:D:282:ARG:NH2	2.36	0.40
1:C:265:GLU:HB3	2:C:350:HOH:O	2.21	0.40
1:D:188:GLN:OE1	1:D:235:ALA:CB	2.66	0.40
1:A:278:ASN:CG	1:B:65:GLY:HA3	2.41	0.40
1:D:234:ALA:O	1:D:235:ALA:CB	2.69	0.40

All (47) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:NH2	1:C:254:THR:CB[2_553]	0.14	2.06
1:B:254:THR:OG1	1:D:185:ARG:NE[4_554]	0.63	1.57
1:B:254:THR:C	1:D:185:ARG:NH1[4_554]	0.70	1.50
1:C:185:ARG:NH1	1:C:254:THR:C[2_553]	0.70	1.50
1:B:252:ASP:CG	1:D:102:ARG:NH2[4_554]	0.76	1.44
1:C:185:ARG:NE	1:C:254:THR:CG2[2_553]	0.77	1.43
1:B:252:ASP:CG	1:D:102:ARG:CZ[4_554]	0.83	1.37
1:B:254:THR:CA	1:D:185:ARG:NH2[4_554]	0.89	1.31
1:B:252:ASP:CB	1:D:102:ARG:NH1[4_554]	0.91	1.29
1:C:185:ARG:NH1	1:C:254:THR:O[2_553]	0.98	1.22
1:C:185:ARG:CZ	1:C:254:THR:CG2[2_553]	1.01	1.19
1:B:252:ASP:OD1	1:D:102:ARG:NH2[4_554]	1.05	1.15
1:B:254:THR:CB	1:D:185:ARG:CZ[4_554]	1.14	1.06
1:B:254:THR:CB	1:D:185:ARG:NH2[4_554]	1.16	1.04
1:B:252:ASP:OD2	1:D:102:ARG:NH2[4_554]	1.19	1.01
1:B:254:THR:CA	1:D:185:ARG:CZ[4_554]	1.22	0.98
1:C:185:ARG:CZ	1:C:254:THR:CB[2_553]	1.28	0.92
1:B:252:ASP:OD1	1:D:102:ARG:CZ[4_554]	1.29	0.91
1:B:254:THR:OG1	1:D:185:ARG:CZ[4_554]	1.32	0.88
1:B:254:THR:O	1:D:185:ARG:NH1[4_554]	1.33	0.87
1:B:254:THR:CB	1:D:185:ARG:NE[4_554]	1.36	0.84
1:B:254:THR:N	1:D:185:ARG:NH2[4_554]	1.36	0.84
1:B:255:ILE:N	1:D:185:ARG:NH1[4_554]	1.39	0.81
1:C:185:ARG:NH2	1:C:254:THR:OG1[2_553]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:NH2	1:C:254:THR:CA[2_553]	1.54	0.66
1:B:254:THR:C	1:D:185:ARG:CZ[4_554]	1.55	0.65
1:B:252:ASP:CG	1:D:102:ARG:NH1[4_554]	1.56	0.64
1:C:185:ARG:NH1	1:C:254:THR:CA[2_553]	1.59	0.61
1:C:185:ARG:NH2	1:C:254:THR:CG2[2_553]	1.60	0.60
1:B:252:ASP:CA	1:D:102:ARG:NH1[4_554]	1.61	0.59
1:B:252:ASP:OD2	1:D:102:ARG:CZ[4_554]	1.61	0.59
1:A:178:ARG:NH2	1:A:178:ARG:NH2[2_554]	1.66	0.54
1:C:185:ARG:CZ	1:C:254:THR:CA[2_553]	1.70	0.50
1:B:254:THR:CG2	1:D:185:ARG:NH2[4_554]	1.72	0.48
1:B:252:ASP:CB	1:D:102:ARG:CZ[4_554]	1.76	0.44
1:B:254:THR:OG1	1:D:185:ARG:CD[4_554]	1.82	0.38
1:B:254:THR:CA	1:D:185:ARG:NH1[4_554]	1.85	0.35
1:C:185:ARG:CZ	1:C:254:THR:C[2_553]	1.85	0.35
1:C:185:ARG:NH1	1:C:255:ILE:N[2_553]	1.93	0.27
1:C:178:ARG:NH1	1:C:253:GLU:OE2[2_553]	2.04	0.16
1:B:252:ASP:OD1	1:D:102:ARG:NE[4_554]	2.08	0.12
1:B:252:ASP:CG	1:D:102:ARG:NE[4_554]	2.08	0.12
1:B:254:THR:O	1:D:185:ARG:CZ[4_554]	2.12	0.08
1:B:254:THR:OG1	1:D:185:ARG:NH2[4_554]	2.14	0.06
1:A:185:ARG:NH1	1:A:254:THR:CG2[2_554]	2.15	0.05
1:B:107:ARG:NH1	1:D:170:GLN:OE1[4_554]	2.15	0.05
1:C:185:ARG:CZ	1:C:254:THR:O[2_553]	2.15	0.05

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	229/249 (92%)	222 (97%)	7 (3%)	0	100	100
1	B	230/249 (92%)	220 (96%)	10 (4%)	0	100	100
1	C	228/249 (92%)	220 (96%)	7 (3%)	1 (0%)	34	41
1	D	230/249 (92%)	225 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	917/996 (92%)	887 (97%)	29 (3%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	105	GLY

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	190/199 (96%)	187 (98%)	3 (2%)	62 77
1	B	191/199 (96%)	182 (95%)	9 (5%)	26 36
1	C	190/199 (96%)	188 (99%)	2 (1%)	73 85
1	D	191/199 (96%)	185 (97%)	6 (3%)	40 55
All	All	762/796 (96%)	742 (97%)	20 (3%)	46 62

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASP
1	A	182	SER
1	A	217	LYS
1	B	71	GLN
1	B	75	ARG
1	B	81	SER
1	B	99	GLU
1	B	102	ARG
1	B	106	ASP
1	B	188	GLN
1	B	282	ARG
1	B	286	LEU
1	C	239	ILE
1	C	282	ARG

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Mol	Chain	Res	Type
1	D	74	SER
1	D	100	ARG
1	D	113	ARG
1	D	148	SER
1	D	150	ARG
1	D	182	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	149	GLN
1	A	167	HIS
1	B	285	ASN
1	C	145	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 monosaccharides 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 ⓘ

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, 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	231/249 (92%)	0.28	12 (5%) 27 34	26, 40, 75, 124	1 (0%)
1	B	232/249 (93%)	0.77	33 (14%) 2 4	25, 44, 112, 166	1 (0%)
1	C	230/249 (92%)	0.49	18 (7%) 13 17	26, 40, 85, 135	1 (0%)
1	D	232/249 (93%)	0.35	13 (5%) 24 31	27, 41, 80, 193	0
All	All	925/996 (92%)	0.48	76 (8%) 11 15	25, 41, 94, 193	3 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	9.6
1	B	105	GLY	7.7
1	C	288	ALA	7.0
1	C	105	GLY	6.9
1	B	58	THR	6.8
1	D	104	ASP	6.5
1	C	103	GLY	6.5
1	B	236	GLY	6.3
1	B	288	ALA	5.9
1	D	105	GLY	5.4
1	B	59	GLY	5.3
1	B	97	ARG	5.2
1	D	107	ARG	5.0
1	B	235	ALA	4.8
1	C	204	ALA	4.8
1	C	106	ASP	4.6
1	B	204	ALA	4.4
1	B	289	ILE	4.3
1	D	102	ARG	4.2
1	C	289	ILE	4.2
1	A	106	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	104	ASP	4.1
1	B	285	ASN	4.0
1	C	102	ARG	3.9
1	B	107	ARG	3.9
1	A	147	TRP	3.8
1	B	103	GLY	3.6
1	C	147	TRP	3.6
1	C	235	ALA	3.5
1	B	102	ARG	3.5
1	B	284	GLY	3.4
1	C	101	LEU	3.3
1	D	147	TRP	3.3
1	A	290	THR	3.3
1	B	99	GLU	3.1
1	B	147	TRP	3.1
1	A	62	ALA	3.1
1	A	64	TYR	3.1
1	C	110	ALA	3.1
1	A	107	ARG	3.1
1	B	106	ASP	3.0
1	B	110	ALA	3.0
1	B	281	ALA	3.0
1	D	204	ALA	3.0
1	B	287	LYS	3.0
1	B	101	LEU	2.9
1	B	238	GLN	2.9
1	C	107	ARG	2.9
1	C	109	ALA	2.9
1	B	108	SER	2.9
1	A	109	ALA	2.8
1	C	188	GLN	2.7
1	D	235	ALA	2.6
1	A	110	ALA	2.6
1	D	291	ALA	2.6
1	D	106	ASP	2.6
1	C	236	GLY	2.6
1	B	280	LEU	2.5
1	D	60	GLU	2.4
1	D	110	ALA	2.4
1	A	235	ALA	2.3
1	B	100	ARG	2.3
1	C	100	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	205	ASP	2.3
1	B	279	ILE	2.3
1	B	283	ALA	2.2
1	B	286	LEU	2.2
1	A	282	ARG	2.2
1	A	105	GLY	2.2
1	D	69	VAL	2.1
1	D	109	ALA	2.1
1	B	188	GLN	2.1
1	C	286	LEU	2.1
1	B	239	ILE	2.1
1	A	104	ASP	2.1
1	B	71	GLN	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 monosaccharides 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.