



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:53 AM UTC

PDB ID : 5ZYT / pdb_00005zyt
Title : Crystal structure of human MGME1 with 3' overhang double strand DNA3
Authors : Yang, C.; Gan, J.
Deposited on : 2018-05-28
Resolution : 2.70 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

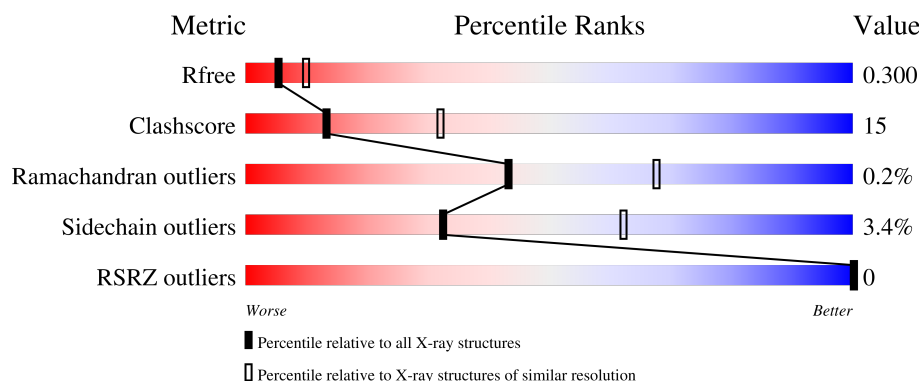
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

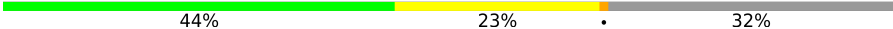
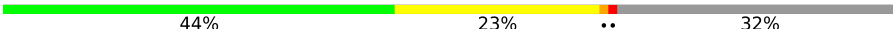
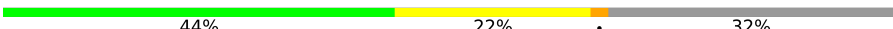
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	324	 44% 23% 32%
1	B	324	 44% 23% 32%
1	C	324	 44% 22% 32%
1	D	324	 45% 21% 32%
2	E	18	 11% 33% 56%

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Mol	Chain	Length	Quality of chain
2	F	18	17% 44% 39%
2	G	18	44% 50% 6%
2	H	18	17% 33% 50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8036 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 Mitochondrial genome maintenance exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1787	1153	299	326	9			
1	B	219	Total	C	N	O	S	0	0	0
			1782	1150	299	324	9			
1	C	220	Total	C	N	O	S	0	0	0
			1802	1162	303	328	9			
1	D	220	Total	C	N	O	S	0	0	0
			1793	1156	302	326	9			

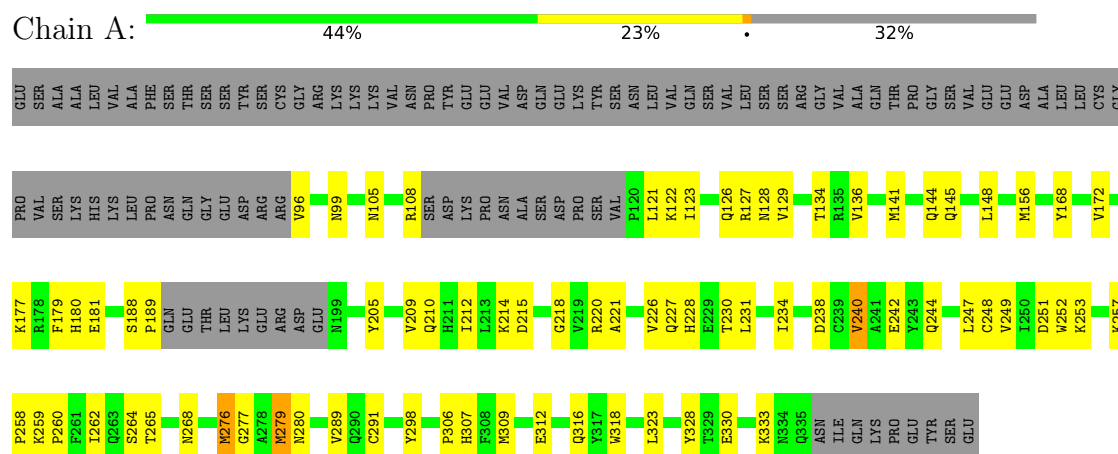
- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*TP*TP*CP*TP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	P	0	0	0
			141	67	17	49	8			
2	F	11	Total	C	N	O	P	0	0	0
			216	106	26	73	11			
2	G	17	Total	C	N	O	P	0	0	0
			336	164	49	107	16			
2	H	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

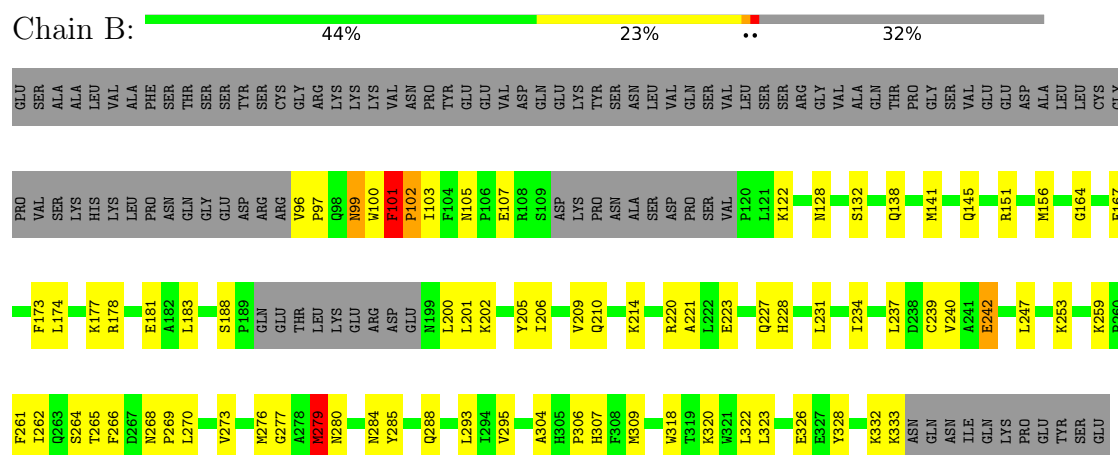
3 Residue-property plots

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.

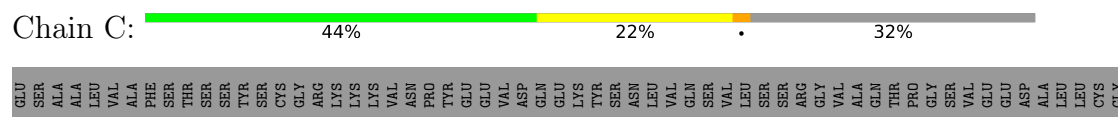
• Molecule 1: Mitochondrial genome maintenance exonuclease 1

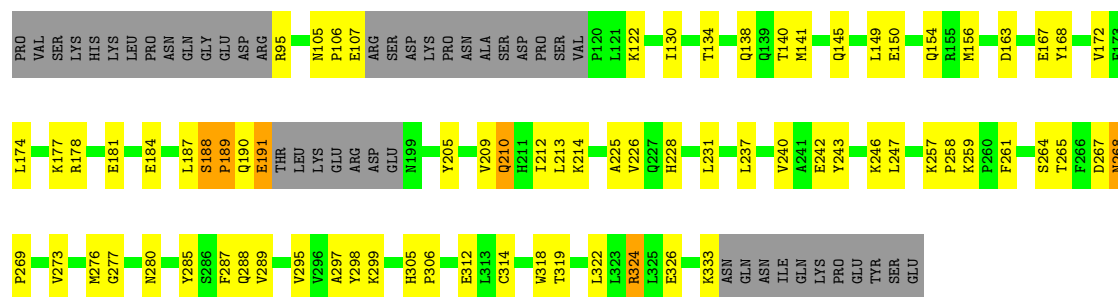


• Molecule 1: Mitochondrial genome maintenance exonuclease 1

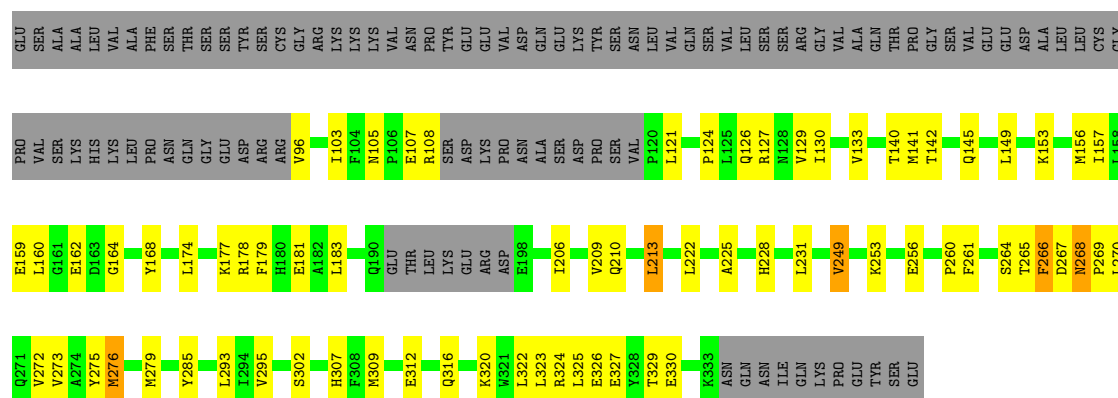


• Molecule 1: Mitochondrial genome maintenance exonuclease 1

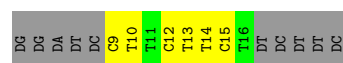




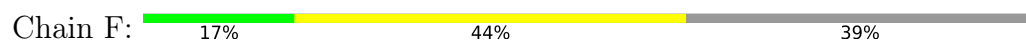
- Molecule 1: Mitochondrial genome maintenance exonuclease 1



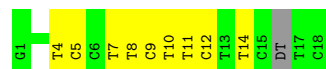
- Molecule 2: DNA (5'-D(P*CP*TP*TP*CP*TP*TP*CP*C)-3')



- Molecule 2: DNA (5'-D(P*CP*TP*TP*CP*TP*TP*CP*C)-3')



- Molecule 2: DNA (5'-D(P*CP*TP*TP*CP*TP*TP*CP*C)-3')



- Molecule 2: DNA (5'-D(P*CP*TP*TP*CP*TP*TP*CP*C)-3')



G1	G2	A3	T7	T8	C9	DT	DT	DC	DC	DT	DT	DC	DC	DT	DT	DC	DC
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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	146.50Å 77.49Å 164.71Å 90.00° 112.40° 90.00°	Depositor
Resolution (Å)	29.96 – 2.70 29.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.4 (29.96-2.70) 73.6 (29.96-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.72Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.249 , 0.296 0.251 , 0.300	Depositor DCC
R_{free} test set	2150 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 19.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8036	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.44% 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 [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	0.65	8/1831 (0.4%)	0.70	0/2481
1	B	0.71	8/1826 (0.4%)	0.80	3/2473 (0.1%)
1	C	0.60	2/1846 (0.1%)	0.79	5/2498 (0.2%)
1	D	0.61	4/1837 (0.2%)	0.71	0/2487
2	E	0.43	0/154	0.69	0/235
2	F	0.46	0/237	0.67	0/362
2	G	0.49	0/371	0.63	0/567
2	H	0.54	0/199	0.70	0/305
All	All	0.63	22/8301 (0.3%)	0.74	8/11408 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	MET	SD-CE	6.95	1.97	1.79
1	A	156	MET	CG-SD	6.81	1.97	1.80
1	A	156	MET	SD-CE	6.58	1.96	1.79
1	B	279	MET	SD-CE	6.53	1.95	1.79
1	A	268	ASN	C-O	-6.44	1.18	1.24
1	D	268	ASN	C-O	-6.41	1.18	1.24
1	B	279	MET	CG-SD	6.40	1.96	1.80
1	B	309	MET	CG-SD	6.33	1.96	1.80
1	A	309	MET	SD-CE	6.07	1.94	1.79
1	D	276	MET	SD-CE	6.04	1.94	1.79
1	D	266	PHE	C-O	-6.01	1.19	1.24
1	C	268	ASN	C-O	-5.92	1.19	1.24
1	D	276	MET	CG-SD	5.88	1.95	1.80
1	A	276	MET	SD-CE	5.81	1.94	1.79
1	B	276	MET	SD-CE	5.76	1.94	1.79
1	C	156	MET	SD-CE	5.64	1.93	1.79
1	B	101	PHE	C-O	-5.59	1.20	1.25
1	B	156	MET	SD-CE	5.58	1.93	1.79
1	B	266	PHE	C-O	-5.54	1.19	1.24
1	A	276	MET	CG-SD	5.52	1.94	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	MET	SD-CE	5.15	1.92	1.79
1	A	309	MET	CG-SD	5.05	1.93	1.80

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	GLN	N-CA-C	7.09	122.06	113.41
1	B	101	PHE	CA-C-N	6.80	128.34	119.84
1	B	101	PHE	C-N-CA	6.80	128.34	119.84
1	B	101	PHE	C-N-CD	-6.37	98.90	125.00
1	C	188	SER	CA-C-N	6.24	127.63	119.84
1	C	188	SER	C-N-CA	6.24	127.63	119.84
1	C	189	PRO	N-CA-C	5.89	124.61	112.47
1	C	188	SER	C-N-CD	-5.58	102.10	125.00

There are no chirality outliers.

There are no planarity outliers.

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	1787	0	1766	58	0
1	B	1782	0	1768	64	0
1	C	1802	0	1794	66	0
1	D	1793	0	1778	51	0
2	E	141	0	81	4	0
2	F	216	0	129	10	0
2	G	336	0	198	7	0
2	H	179	0	104	11	0
All	All	8036	0	7618	231	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 15.

All (231) 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:264:SER:OG	2:F:17:DC:O2	1.81	0.98
2:H:1:DG:H5"	2:H:2:DG:OP2	1.68	0.93
2:E:9:DC:H2"	2:E:10:DT:H5"	1.55	0.89
1:B:220:ARG:HB2	1:B:240:VAL:HG23	1.57	0.86
1:B:262:ILE:O	1:B:265:THR:OG1	1.95	0.83
1:A:127:ARG:NH2	1:B:284:ASN:OD1	2.11	0.83
1:A:323:LEU:HD21	1:B:97:PRO:HG3	1.60	0.82
1:C:188:SER:HB3	1:C:189:PRO:HD2	1.64	0.79
1:B:320:LYS:HA	1:B:323:LEU:HD12	1.65	0.79
1:B:200:LEU:HD21	1:C:191:GLU:HB3	1.64	0.77
1:A:227:GLN:HG3	1:A:234:ILE:HG22	1.68	0.75
1:D:124:PRO:HD2	1:D:127:ARG:HG3	1.70	0.74
1:A:248:CYS:HB3	1:A:291:CYS:HB2	1.71	0.71
1:A:218:GLY:O	1:A:220:ARG:NH1	2.24	0.71
1:A:228:HIS:CD2	1:A:231:LEU:H	2.09	0.70
1:C:280:ASN:HD22	1:C:288:GLN:HB2	1.55	0.69
1:B:227:GLN:HB2	1:B:234:ILE:HG22	1.76	0.68
1:B:138:GLN:HA	1:B:141:MET:HE3	1.77	0.67
1:B:201:LEU:HD13	1:C:210:GLN:HG3	1.76	0.67
1:C:273:VAL:HA	1:C:276:MET:HE2	1.76	0.67
1:A:126:GLN:HA	1:A:129:VAL:HG13	1.76	0.66
1:C:280:ASN:ND2	1:C:289:VAL:H	1.93	0.65
1:D:267:ASP:OD2	1:D:324:ARG:NH2	2.23	0.65
1:C:187:LEU:HD21	1:C:213:LEU:HD11	1.78	0.65
1:C:276:MET:HE3	1:D:103:ILE:HD11	1.78	0.65
1:C:134:THR:O	1:C:138:GLN:HG3	1.97	0.65
1:D:225:ALA:O	1:D:285:TYR:OH	2.15	0.65
1:C:188:SER:CB	1:C:189:PRO:HD2	2.25	0.64
2:G:9:DC:H2"	2:G:10:DT:H5"	1.80	0.64
1:A:323:LEU:CD2	1:B:97:PRO:HG3	2.28	0.64
1:B:210:GLN:NE2	1:C:210:GLN:OE1	2.31	0.63
1:C:228:HIS:HD2	1:C:231:LEU:H	1.46	0.63
1:A:134:THR:OG1	2:E:10:DT:OP2	2.13	0.62
1:C:228:HIS:CD2	1:C:231:LEU:H	2.18	0.62
1:B:221:ALA:HB3	1:B:240:VAL:HG22	1.81	0.62
1:C:225:ALA:O	1:C:285:TYR:OH	2.13	0.62
1:C:228:HIS:CD2	1:C:231:LEU:HB2	2.35	0.61
1:A:122:LYS:HE2	1:B:223:GLU:HB2	1.82	0.61
1:B:177:LYS:O	1:B:181:GLU:HG3	2.00	0.61
1:D:130:ILE:H	1:D:130:ILE:HD12	1.65	0.61
1:C:177:LYS:O	1:C:181:GLU:HG3	2.01	0.61
1:B:261:PHE:O	1:B:264:SER:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LYS:HD3	1:D:268:ASN:OD1	2.01	0.61
1:C:149:LEU:HD11	2:G:14:DT:C6	2.36	0.61
1:A:128:ASN:HB3	1:B:227:GLN:OE1	2.00	0.60
1:C:212:ILE:HD11	1:C:306:PRO:HD3	1.83	0.60
1:D:261:PHE:O	1:D:264:SER:HB2	2.02	0.60
1:C:276:MET:HE1	1:C:314:CYS:HB3	1.84	0.59
1:A:323:LEU:HD21	1:B:97:PRO:CG	2.32	0.59
1:B:132:SER:CB	2:F:10:DT:H3'	2.33	0.59
1:A:221:ALA:HB3	1:A:240:VAL:HG23	1.85	0.58
1:A:276:MET:HE2	1:B:103:ILE:HD11	1.84	0.58
1:C:277:GLY:HA3	1:C:318:TRP:CZ3	2.39	0.58
1:D:179:PHE:CZ	1:D:183:LEU:HD11	2.38	0.57
1:D:142:THR:HG23	1:D:145:GLN:H	1.69	0.57
1:C:105:ASN:HB3	1:C:107:GLU:H	1.68	0.57
1:C:150:GLU:O	1:C:154:GLN:HG2	2.05	0.57
1:A:177:LYS:O	1:A:181:GLU:HG2	2.05	0.57
1:C:280:ASN:HD21	1:C:289:VAL:H	1.50	0.57
1:C:242:GLU:HA	1:C:247:LEU:HA	1.85	0.56
1:C:163:ASP:HB3	1:C:167:GLU:OE1	2.05	0.56
1:A:212:ILE:HD11	1:A:306:PRO:HG3	1.88	0.55
1:C:168:TYR:O	1:C:172:VAL:HG23	2.07	0.55
1:A:141:MET:HE3	1:A:145:GLN:HG2	1.89	0.55
1:A:258:PRO:HA	1:A:298:TYR:CE1	2.41	0.55
1:B:277:GLY:HA3	1:B:318:TRP:CZ3	2.42	0.55
1:A:108:ARG:HG3	1:B:288:GLN:HB3	1.87	0.55
1:C:258:PRO:HA	1:C:298:TYR:CE1	2.41	0.55
1:C:298:TYR:OH	1:C:305:HIS:CD2	2.60	0.54
1:B:268:ASN:N	1:B:269:PRO:CD	2.71	0.54
1:B:268:ASN:N	1:B:269:PRO:HD2	2.22	0.54
1:C:322:LEU:O	1:C:326:GLU:HG3	2.06	0.54
1:D:206:ILE:HA	1:D:209:VAL:HG22	1.89	0.54
1:C:105:ASN:HB3	1:C:107:GLU:N	2.23	0.53
1:B:164:GLY:O	1:B:167:GLU:HB2	2.08	0.53
1:D:177:LYS:HE3	1:D:181:GLU:OE2	2.08	0.53
1:B:242:GLU:HA	1:B:247:LEU:HA	1.90	0.53
1:D:105:ASN:O	1:D:107:GLU:N	2.42	0.53
1:D:145:GLN:HE21	2:H:7:DT:H3	1.57	0.53
2:E:14:DT:H2''	2:E:15:DC:H5'	1.91	0.53
1:C:184:GLU:O	1:C:188:SER:OG	2.26	0.52
1:A:276:MET:HG2	1:A:289:VAL:HG13	1.91	0.52
2:F:11:DC:H2''	2:F:12:DT:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:SER:HB3	1:C:189:PRO:CD	2.35	0.52
1:D:141:MET:HE1	1:D:149:LEU:HD12	1.91	0.52
1:A:141:MET:CE	1:A:145:GLN:HG2	2.40	0.52
1:B:205:TYR:O	1:B:209:VAL:HG22	2.09	0.52
1:A:228:HIS:ND1	1:A:231:LEU:HB2	2.25	0.52
1:D:322:LEU:O	1:D:326:GLU:HG3	2.10	0.52
1:C:298:TYR:OH	1:C:305:HIS:HD2	1.93	0.52
2:F:9:DT:H2'	2:F:10:DT:H71	1.92	0.52
1:D:168:TYR:OH	1:D:256:GLU:OE2	2.24	0.51
1:D:276:MET:O	1:D:279:MET:N	2.43	0.51
1:A:215:ASP:OD2	1:A:244:GLN:NE2	2.40	0.51
1:B:145:GLN:HG3	2:F:15:DT:N3	2.26	0.51
1:A:280:ASN:O	1:B:105:ASN:HB2	2.11	0.51
2:H:1:DG:H2'	2:H:1:DG:N3	2.24	0.51
1:A:220:ARG:HD2	1:A:247:LEU:HD11	1.91	0.51
1:A:228:HIS:CG	1:A:231:LEU:HB2	2.45	0.51
1:A:108:ARG:NH1	1:B:285:TYR:O	2.43	0.51
1:C:237:LEU:HD13	1:C:240:VAL:HG23	1.93	0.51
1:B:206:ILE:O	1:B:210:GLN:HG3	2.12	0.50
1:C:268:ASN:N	1:C:269:PRO:CD	2.75	0.50
1:B:280:ASN:HB3	1:B:288:GLN:HB2	1.93	0.50
1:D:312:GLU:O	1:D:316:GLN:HG3	2.12	0.50
1:C:174:LEU:HD21	1:C:178:ARG:NH2	2.26	0.50
1:D:206:ILE:O	1:D:210:GLN:HG3	2.11	0.50
1:B:99:ASN:ND2	1:B:99:ASN:N	2.59	0.50
1:C:141:MET:HE3	1:C:145:GLN:HG2	1.93	0.50
1:A:144:GLN:O	1:A:148:LEU:HG	2.12	0.49
1:D:249:VAL:HG22	1:D:272:VAL:HG13	1.94	0.49
1:B:253:LYS:HD3	2:F:13:DT:OP2	2.13	0.49
1:C:318:TRP:HB2	1:D:103:ILE:HD12	1.94	0.49
1:C:95:ARG:NH2	1:D:327:GLU:OE1	2.46	0.49
1:D:145:GLN:HG3	2:H:7:DT:N3	2.28	0.49
1:D:272:VAL:O	1:D:276:MET:HG3	2.13	0.48
2:H:2:DG:H2''	2:H:3:DA:O4'	2.13	0.48
1:A:262:ILE:O	1:A:265:THR:OG1	2.32	0.48
1:C:122:LYS:HG3	1:D:222:LEU:O	2.12	0.48
1:C:312:GLU:N	1:C:312:GLU:OE1	2.46	0.48
1:B:228:HIS:NE2	1:B:231:LEU:HD12	2.29	0.48
1:D:133:VAL:HG12	2:H:3:DA:OP1	2.14	0.48
2:H:2:DG:H2''	2:H:3:DA:O5'	2.14	0.48
2:F:9:DT:H2'	2:F:10:DT:C7	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:HIS:CE1	1:A:231:LEU:HB2	2.49	0.47
1:D:157:ILE:HG23	1:D:162:GLU:HA	1.97	0.47
1:D:133:VAL:HG11	1:D:275:TYR:CE1	2.49	0.47
1:A:136:VAL:HA	1:A:328:TYR:CD2	2.51	0.47
1:A:318:TRP:HB2	1:B:103:ILE:HD12	1.96	0.47
1:C:141:MET:HE1	1:C:149:LEU:HD22	1.97	0.47
1:D:153:LYS:O	1:D:157:ILE:HG13	2.15	0.47
1:B:210:GLN:O	1:B:214:LYS:HG3	2.14	0.46
1:C:210:GLN:O	1:C:214:LYS:HG3	2.15	0.46
1:D:160:LEU:HB3	1:D:164:GLY:HA3	1.97	0.46
1:C:149:LEU:HD11	2:G:14:DT:C5	2.50	0.46
1:C:205:TYR:CZ	1:C:299:LYS:HB2	2.50	0.46
1:C:243:TYR:O	1:C:246:LYS:HG2	2.14	0.46
1:B:202:LYS:HE2	1:C:214:LYS:O	2.15	0.46
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.72	0.46
1:A:251:ASP:OD2	1:A:253:LYS:NZ	2.46	0.46
1:A:312:GLU:O	1:A:316:GLN:HG3	2.15	0.46
2:G:7:DT:H2''	2:G:8:DT:H5'	1.97	0.46
1:B:328:TYR:O	1:B:332:LYS:HG2	2.16	0.46
1:C:267:ASP:OD2	1:C:324:ARG:NH2	2.49	0.46
1:D:121:LEU:HD23	1:D:121:LEU:HA	1.74	0.46
1:D:293:LEU:HD12	1:D:307:HIS:O	2.16	0.46
1:A:210:GLN:O	1:A:214:LYS:HG3	2.16	0.45
1:C:257:LYS:HB2	1:C:257:LYS:HE2	1.48	0.45
1:A:105:ASN:ND2	1:A:108:ARG:HE	2.13	0.45
1:B:332:LYS:C	1:B:333:LYS:HG3	2.41	0.45
1:C:287:PHE:O	1:D:108:ARG:NH1	2.47	0.45
1:B:270:LEU:HA	1:B:273:VAL:HG22	1.97	0.45
2:E:12:DC:H2'	2:E:13:DT:C6	2.51	0.45
1:A:330:GLU:HA	1:A:333:LYS:HE3	1.97	0.45
1:C:140:THR:OG1	1:C:324:ARG:NH1	2.37	0.45
1:C:268:ASN:HB2	1:C:269:PRO:HD3	1.98	0.45
1:A:179:PHE:HZ	1:A:209:VAL:HG21	1.82	0.45
1:A:209:VAL:HG11	1:A:252:TRP:CZ3	2.51	0.45
1:B:101:PHE:HA	1:B:102:PRO:HD3	1.56	0.45
1:D:249:VAL:CG2	1:D:272:VAL:HG13	2.47	0.45
1:A:212:ILE:CD1	1:A:306:PRO:HG3	2.47	0.45
1:C:210:GLN:HE21	1:C:210:GLN:HB2	1.60	0.45
1:A:126:GLN:O	1:A:129:VAL:HG22	2.17	0.44
1:D:140:THR:HG21	1:D:324:ARG:O	2.17	0.44
1:A:205:TYR:O	1:A:209:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:PRO:HG2	1:D:261:PHE:CE1	2.52	0.44
1:A:105:ASN:HD22	1:A:108:ARG:HE	1.65	0.44
1:D:270:LEU:HA	1:D:273:VAL:HG22	1.99	0.44
1:C:259:LYS:HE3	1:C:265:THR:HG22	1.99	0.44
1:B:237:LEU:HD13	1:B:240:VAL:HG13	1.99	0.44
1:B:173:PHE:CD1	2:F:12:DT:C2	3.06	0.44
1:D:145:GLN:HG3	2:H:7:DT:H3	1.83	0.44
1:C:149:LEU:CD1	2:G:14:DT:C6	3.01	0.43
1:A:249:VAL:HG23	1:A:289:VAL:HG11	1.99	0.43
1:C:168:TYR:CE1	1:C:172:VAL:HG21	2.54	0.43
1:C:212:ILE:HD13	1:C:295:VAL:HG13	2.00	0.43
1:A:220:ARG:HH12	1:A:242:GLU:HG3	1.82	0.43
1:A:180:HIS:HD2	1:A:238:ASP:OD1	2.02	0.43
1:B:259:LYS:HE3	2:F:16:DT:O4	2.18	0.43
1:B:304:ALA:O	1:B:306:PRO:HD3	2.19	0.43
1:C:261:PHE:O	1:C:264:SER:HB2	2.18	0.43
1:D:266:PHE:CZ	2:H:8:DT:C2	3.07	0.43
1:A:248:CYS:HB3	1:A:291:CYS:CB	2.46	0.43
1:B:328:TYR:CE1	1:B:332:LYS:HE3	2.54	0.43
1:D:126:GLN:O	1:D:129:VAL:HG22	2.19	0.43
1:A:277:GLY:HA2	1:B:103:ILE:O	2.19	0.42
1:B:151:ARG:HA	1:B:151:ARG:NE	2.34	0.42
1:B:322:LEU:O	1:B:326:GLU:HG3	2.19	0.42
1:D:264:SER:OG	2:H:9:DC:O2	2.37	0.42
1:A:123:ILE:HD12	1:A:127:ARG:NH1	2.34	0.42
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.86	0.42
1:B:279:MET:HE2	1:B:279:MET:HB3	1.75	0.42
1:B:240:VAL:HG23	1:B:240:VAL:O	2.19	0.42
1:D:325:LEU:O	1:D:329:THR:HG23	2.18	0.42
1:B:228:HIS:CD2	1:B:231:LEU:HD12	2.54	0.42
1:B:293:LEU:HG	1:B:295:VAL:HG23	2.01	0.42
1:C:209:VAL:HG13	1:C:297:ALA:HB2	2.02	0.42
1:B:277:GLY:HA3	1:B:318:TRP:CH2	2.54	0.42
1:A:231:LEU:HA	1:A:231:LEU:HD23	1.80	0.42
1:B:200:LEU:CD2	1:C:191:GLU:HB3	2.44	0.42
1:B:259:LYS:O	1:B:307:HIS:HE1	2.02	0.42
1:C:246:LYS:HG2	1:C:246:LYS:H	1.66	0.42
1:C:276:MET:CE	1:D:103:ILE:HD11	2.47	0.42
1:D:159:GLU:C	1:D:160:LEU:HD12	2.45	0.42
2:G:4:DT:H2''	2:G:5:DC:C6	2.55	0.42
1:A:168:TYR:O	1:A:172:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.88	0.41
1:D:228:HIS:CG	1:D:231:LEU:HB2	2.55	0.41
1:C:174:LEU:HD21	1:C:178:ARG:HH21	1.85	0.41
2:G:11:DT:H72	2:G:12:DC:C4	2.55	0.41
1:A:260:PRO:O	1:A:307:HIS:HE1	2.02	0.41
1:B:174:LEU:O	1:B:178:ARG:HG3	2.21	0.41
1:D:320:LYS:HA	1:D:323:LEU:HD12	2.02	0.41
1:A:226:VAL:HG11	1:A:279:MET:HB2	2.03	0.41
1:A:188:SER:HA	1:A:189:PRO:HD3	1.87	0.41
1:B:228:HIS:CG	1:B:231:LEU:HB2	2.56	0.41
1:C:276:MET:O	1:C:277:GLY:C	2.63	0.41
1:D:209:VAL:O	1:D:213:LEU:HB2	2.21	0.41
1:D:265:THR:OG1	1:D:269:PRO:HD3	2.21	0.41
1:D:326:GLU:O	1:D:330:GLU:HB2	2.21	0.41
1:B:105:ASN:CG	1:B:107:GLU:HG2	2.46	0.40
1:D:174:LEU:O	1:D:178:ARG:HG3	2.20	0.40
2:H:2:DG:C6	2:H:3:DA:C6	3.09	0.40
1:A:228:HIS:NE2	1:A:230:THR:OG1	2.51	0.40
1:A:259:LYS:HE3	1:A:264:SER:O	2.22	0.40
1:B:99:ASN:N	1:B:99:ASN:HD22	2.18	0.40
1:D:156:MET:HE3	1:D:156:MET:HB3	1.72	0.40
1:A:249:VAL:HG21	1:A:276:MET:HG3	2.02	0.40
1:B:122:LYS:HB2	1:B:122:LYS:HE2	1.74	0.40
1:B:145:GLN:HG3	2:F:15:DT:H3	1.86	0.40
1:B:220:ARG:HG3	1:B:247:LEU:HD11	2.04	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	214/324 (66%)	206 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/324 (66%)	206 (97%)	6 (3%)	1 (0%)	24	48
1	C	214/324 (66%)	206 (96%)	7 (3%)	1 (0%)	24	48
1	D	214/324 (66%)	204 (95%)	10 (5%)	0	100	100
All	All	855/1296 (66%)	822 (96%)	31 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	PRO
1	C	106	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/294 (67%)	194 (98%)	4 (2%)	48	76
1	B	198/294 (67%)	188 (95%)	10 (5%)	21	48
1	C	201/294 (68%)	194 (96%)	7 (4%)	32	61
1	D	199/294 (68%)	193 (97%)	6 (3%)	36	66
All	All	796/1176 (68%)	769 (97%)	27 (3%)	32	62

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	99	ASN
1	A	240	VAL
1	A	257	LYS
1	B	96	VAL
1	B	99	ASN
1	B	100	TRP
1	B	101	PHE
1	B	128	ASN

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Mol	Chain	Res	Type
1	B	183	LEU
1	B	188	SER
1	B	239	CYS
1	B	242	GLU
1	B	279	MET
1	C	130	ILE
1	C	191	GLU
1	C	210	GLN
1	C	226	VAL
1	C	319	THR
1	C	324	ARG
1	C	333	LYS
1	D	96	VAL
1	D	213	LEU
1	D	249	VAL
1	D	295	VAL
1	D	302	SER
1	D	309	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	99	ASN
1	A	199	ASN
1	A	271	GLN
1	A	280	ASN
1	B	99	ASN
1	B	139	GLN
1	B	210	GLN
1	C	210	GLN
1	C	228	HIS
1	C	271	GLN
1	C	280	ASN
1	C	290	GLN
1	C	305	HIS
1	D	99	ASN
1	D	126	GLN
1	D	138	GLN
1	D	154	GLN
1	D	210	GLN
1	D	316	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	220/324 (67%)	-1.34	0 100 100	25, 41, 64, 84	0
1	B	219/324 (67%)	-1.42	0 100 100	28, 42, 62, 72	0
1	C	220/324 (67%)	-1.41	0 100 100	24, 39, 63, 77	0
1	D	220/324 (67%)	-1.36	0 100 100	34, 46, 60, 69	0
2	E	8/18 (44%)	-1.55	0 100 100	37, 61, 72, 94	0
2	F	11/18 (61%)	-1.32	0 100 100	38, 51, 115, 116	0
2	G	17/18 (94%)	-1.29	0 100 100	37, 57, 97, 99	0
2	H	9/18 (50%)	-1.50	0 100 100	42, 50, 71, 74	0
All	All	924/1368 (67%)	-1.38	0 100 100	24, 43, 64, 116	0

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.