



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:26 AM UTC

PDB ID : 8XLA / pdb_00008xla
Title : Mismatch Repair Complex
Authors : Nirwal, S.; Nair, D.T.
Deposited on : 2023-12-25
Resolution : 3.50 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

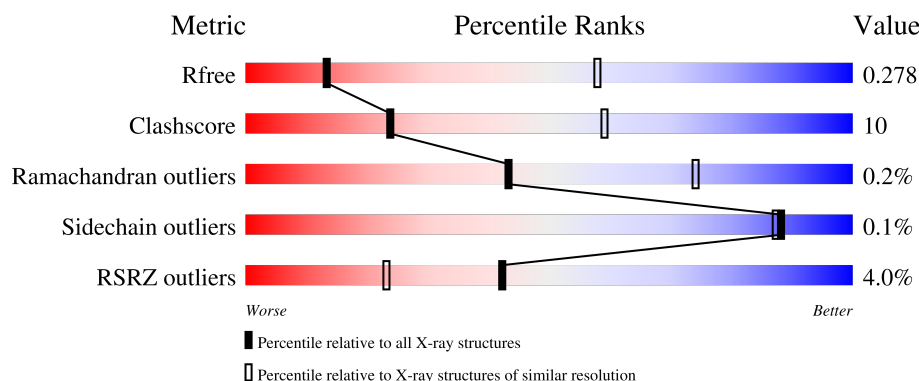
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	387	
1	B	387	
1	E	387	
1	F	387	
2	D	220	

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Mol	Chain	Length	Quality of chain
2	Y	220	10% 45% 39% • 15%
2	Z	220	6% 62% 22% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15581 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2912	1847	505	547	13			
1	B	366	Total	C	N	O	S	0	0	0
			2865	1819	495	539	12			
1	E	367	Total	C	N	O	S	0	0	0
			2874	1824	498	539	13			
1	F	367	Total	C	N	O	S	0	0	0
			2869	1821	496	539	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q5FAJ1
A	-19	GLY	-	expression tag	UNP Q5FAJ1
A	-18	SER	-	expression tag	UNP Q5FAJ1
A	-17	SER	-	expression tag	UNP Q5FAJ1
A	-16	HIS	-	expression tag	UNP Q5FAJ1
A	-15	HIS	-	expression tag	UNP Q5FAJ1
A	-14	HIS	-	expression tag	UNP Q5FAJ1
A	-13	HIS	-	expression tag	UNP Q5FAJ1
A	-12	HIS	-	expression tag	UNP Q5FAJ1
A	-11	HIS	-	expression tag	UNP Q5FAJ1
A	-10	SER	-	expression tag	UNP Q5FAJ1
A	-9	SER	-	expression tag	UNP Q5FAJ1
A	-8	GLY	-	expression tag	UNP Q5FAJ1
A	-7	LEU	-	expression tag	UNP Q5FAJ1
A	-6	VAL	-	expression tag	UNP Q5FAJ1
A	-5	PRO	-	expression tag	UNP Q5FAJ1
A	-4	ARG	-	expression tag	UNP Q5FAJ1
A	-3	GLY	-	expression tag	UNP Q5FAJ1
A	-2	SER	-	expression tag	UNP Q5FAJ1
A	-1	HIS	-	expression tag	UNP Q5FAJ1
B	-19	MET	-	initiating methionine	UNP Q5FAJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q5FAJ1
B	-17	SER	-	expression tag	UNP Q5FAJ1
B	-16	SER	-	expression tag	UNP Q5FAJ1
B	-15	HIS	-	expression tag	UNP Q5FAJ1
B	-14	HIS	-	expression tag	UNP Q5FAJ1
B	-13	HIS	-	expression tag	UNP Q5FAJ1
B	-12	HIS	-	expression tag	UNP Q5FAJ1
B	-11	HIS	-	expression tag	UNP Q5FAJ1
B	-10	HIS	-	expression tag	UNP Q5FAJ1
B	-9	SER	-	expression tag	UNP Q5FAJ1
B	-8	SER	-	expression tag	UNP Q5FAJ1
B	-7	GLY	-	expression tag	UNP Q5FAJ1
B	-6	LEU	-	expression tag	UNP Q5FAJ1
B	-5	VAL	-	expression tag	UNP Q5FAJ1
B	-4	PRO	-	expression tag	UNP Q5FAJ1
B	-3	ARG	-	expression tag	UNP Q5FAJ1
B	-2	GLY	-	expression tag	UNP Q5FAJ1
B	-1	SER	-	expression tag	UNP Q5FAJ1
B	0	HIS	-	expression tag	UNP Q5FAJ1
E	-20	MET	-	initiating methionine	UNP Q5FAJ1
E	-19	GLY	-	expression tag	UNP Q5FAJ1
E	-18	SER	-	expression tag	UNP Q5FAJ1
E	-17	SER	-	expression tag	UNP Q5FAJ1
E	-16	HIS	-	expression tag	UNP Q5FAJ1
E	-15	HIS	-	expression tag	UNP Q5FAJ1
E	-14	HIS	-	expression tag	UNP Q5FAJ1
E	-13	HIS	-	expression tag	UNP Q5FAJ1
E	-12	HIS	-	expression tag	UNP Q5FAJ1
E	-11	HIS	-	expression tag	UNP Q5FAJ1
E	-10	SER	-	expression tag	UNP Q5FAJ1
E	-9	SER	-	expression tag	UNP Q5FAJ1
E	-8	GLY	-	expression tag	UNP Q5FAJ1
E	-7	LEU	-	expression tag	UNP Q5FAJ1
E	-6	VAL	-	expression tag	UNP Q5FAJ1
E	-5	PRO	-	expression tag	UNP Q5FAJ1
E	-4	ARG	-	expression tag	UNP Q5FAJ1
E	-3	GLY	-	expression tag	UNP Q5FAJ1
E	-2	SER	-	expression tag	UNP Q5FAJ1
E	-1	HIS	-	expression tag	UNP Q5FAJ1
F	-20	MET	-	initiating methionine	UNP Q5FAJ1
F	-19	GLY	-	expression tag	UNP Q5FAJ1
F	-18	SER	-	expression tag	UNP Q5FAJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	SER	-	expression tag	UNP Q5FAJ1
F	-16	HIS	-	expression tag	UNP Q5FAJ1
F	-15	HIS	-	expression tag	UNP Q5FAJ1
F	-14	HIS	-	expression tag	UNP Q5FAJ1
F	-13	HIS	-	expression tag	UNP Q5FAJ1
F	-12	HIS	-	expression tag	UNP Q5FAJ1
F	-11	HIS	-	expression tag	UNP Q5FAJ1
F	-10	SER	-	expression tag	UNP Q5FAJ1
F	-9	SER	-	expression tag	UNP Q5FAJ1
F	-8	GLY	-	expression tag	UNP Q5FAJ1
F	-7	LEU	-	expression tag	UNP Q5FAJ1
F	-6	VAL	-	expression tag	UNP Q5FAJ1
F	-5	PRO	-	expression tag	UNP Q5FAJ1
F	-4	ARG	-	expression tag	UNP Q5FAJ1
F	-3	GLY	-	expression tag	UNP Q5FAJ1
F	-2	SER	-	expression tag	UNP Q5FAJ1
F	-1	HIS	-	expression tag	UNP Q5FAJ1

- Molecule 2 is a protein called DNA mismatch repair protein MutL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	186	Total	C	N	O	S	0	0	0
			1409	877	256	266	10			
2	Z	187	Total	C	N	O	S	0	0	0
			1352	839	253	252	8			
2	D	176	Total	C	N	O	S	0	0	0
			1300	812	233	246	9			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	439	THR	-	expression tag	UNP Q5F8M6
Y	440	MET	-	expression tag	UNP Q5F8M6
Y	441	GLY	-	expression tag	UNP Q5F8M6
Y	442	SER	-	expression tag	UNP Q5F8M6
Y	443	SER	-	expression tag	UNP Q5F8M6
Y	444	HIS	-	expression tag	UNP Q5F8M6
Y	445	HIS	-	expression tag	UNP Q5F8M6
Y	446	HIS	-	expression tag	UNP Q5F8M6
Y	447	HIS	-	expression tag	UNP Q5F8M6
Y	448	HIS	-	expression tag	UNP Q5F8M6
Y	449	HIS	-	expression tag	UNP Q5F8M6

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	450	SER	-	expression tag	UNP Q5F8M6
Y	451	SER	-	expression tag	UNP Q5F8M6
Y	452	GLY	-	expression tag	UNP Q5F8M6
Y	453	LEU	-	expression tag	UNP Q5F8M6
Y	454	VAL	-	expression tag	UNP Q5F8M6
Y	455	PRO	-	expression tag	UNP Q5F8M6
Y	456	ARG	-	expression tag	UNP Q5F8M6
Y	457	GLY	-	expression tag	UNP Q5F8M6
Y	458	SER	-	expression tag	UNP Q5F8M6
Y	459	HIS	-	expression tag	UNP Q5F8M6
Z	439	THR	-	expression tag	UNP Q5F8M6
Z	440	MET	-	expression tag	UNP Q5F8M6
Z	441	GLY	-	expression tag	UNP Q5F8M6
Z	442	SER	-	expression tag	UNP Q5F8M6
Z	443	SER	-	expression tag	UNP Q5F8M6
Z	444	HIS	-	expression tag	UNP Q5F8M6
Z	445	HIS	-	expression tag	UNP Q5F8M6
Z	446	HIS	-	expression tag	UNP Q5F8M6
Z	447	HIS	-	expression tag	UNP Q5F8M6
Z	448	HIS	-	expression tag	UNP Q5F8M6
Z	449	HIS	-	expression tag	UNP Q5F8M6
Z	450	SER	-	expression tag	UNP Q5F8M6
Z	451	SER	-	expression tag	UNP Q5F8M6
Z	452	GLY	-	expression tag	UNP Q5F8M6
Z	453	LEU	-	expression tag	UNP Q5F8M6
Z	454	VAL	-	expression tag	UNP Q5F8M6
Z	455	PRO	-	expression tag	UNP Q5F8M6
Z	456	ARG	-	expression tag	UNP Q5F8M6
Z	457	GLY	-	expression tag	UNP Q5F8M6
Z	458	SER	-	expression tag	UNP Q5F8M6
Z	459	HIS	-	expression tag	UNP Q5F8M6
D	439	THR	-	expression tag	UNP Q5F8M6
D	440	MET	-	expression tag	UNP Q5F8M6
D	441	GLY	-	expression tag	UNP Q5F8M6
D	442	SER	-	expression tag	UNP Q5F8M6
D	443	SER	-	expression tag	UNP Q5F8M6
D	444	HIS	-	expression tag	UNP Q5F8M6
D	445	HIS	-	expression tag	UNP Q5F8M6
D	446	HIS	-	expression tag	UNP Q5F8M6
D	447	HIS	-	expression tag	UNP Q5F8M6
D	448	HIS	-	expression tag	UNP Q5F8M6
D	449	HIS	-	expression tag	UNP Q5F8M6

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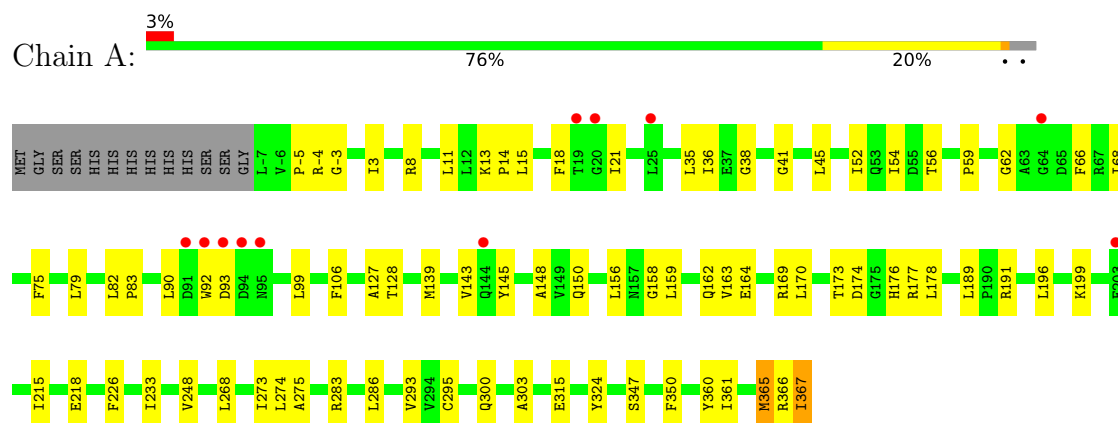
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Chain	Residue	Modelled	Actual	Comment	Reference
D	450	SER	-	expression tag	UNP Q5F8M6
D	451	SER	-	expression tag	UNP Q5F8M6
D	452	GLY	-	expression tag	UNP Q5F8M6
D	453	LEU	-	expression tag	UNP Q5F8M6
D	454	VAL	-	expression tag	UNP Q5F8M6
D	455	PRO	-	expression tag	UNP Q5F8M6
D	456	ARG	-	expression tag	UNP Q5F8M6
D	457	GLY	-	expression tag	UNP Q5F8M6
D	458	SER	-	expression tag	UNP Q5F8M6
D	459	HIS	-	expression tag	UNP Q5F8M6

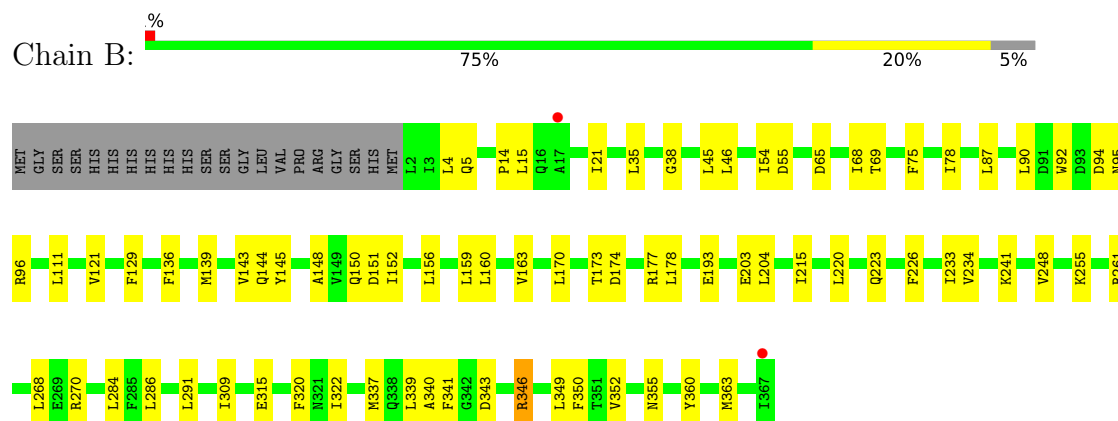
3 Residue-property plots [i](#)

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.

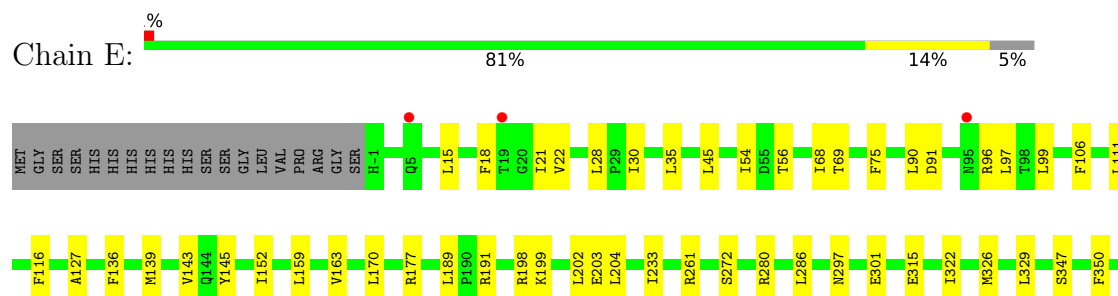
• Molecule 1: Beta sliding clamp

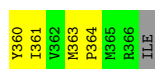


• Molecule 1: Beta sliding clamp

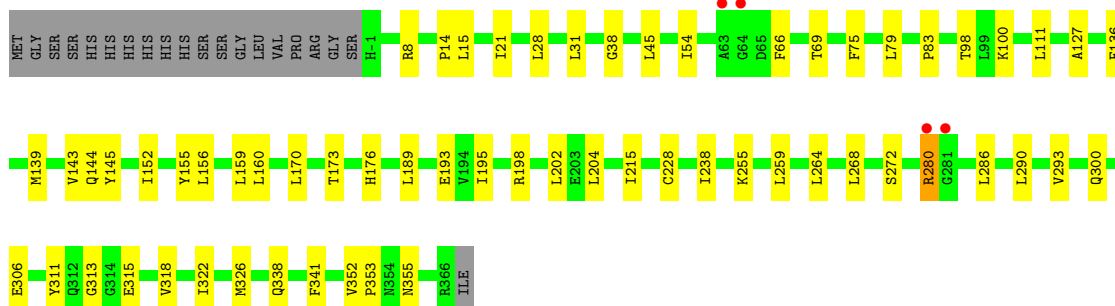
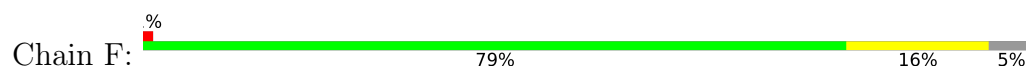


• Molecule 1: Beta sliding clamp

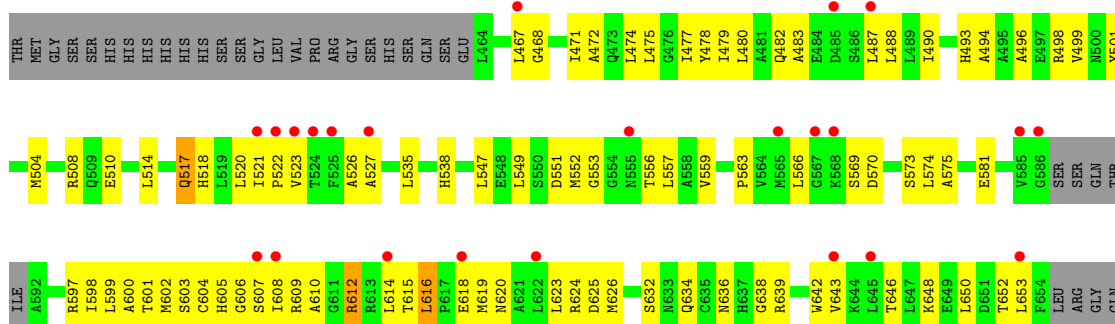




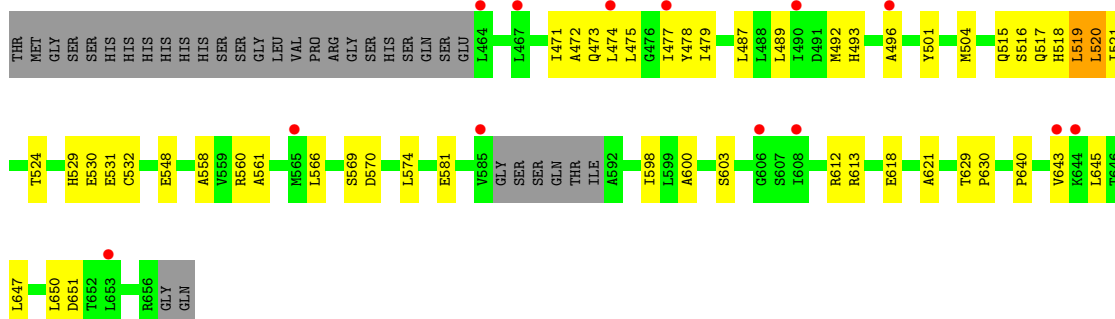
• Molecule 1: Beta sliding clamp



• Molecule 2: DNA mismatch repair protein MutL

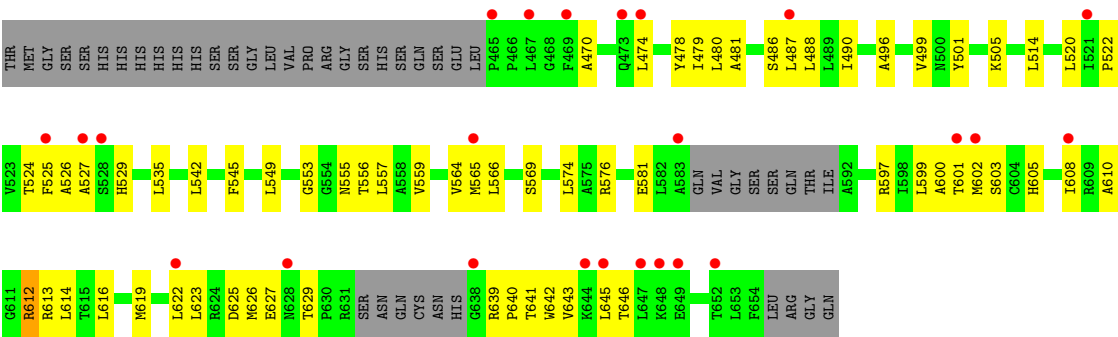


• Molecule 2: DNA mismatch repair protein MutL



• Molecule 2: DNA mismatch repair protein MutL





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	160.75Å 212.04Å 255.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.70 – 3.50 64.70 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (64.70-3.50) 97.7 (64.70-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.267 , 0.280 0.266 , 0.278	Depositor DCC
R_{free} test set	2732 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 93.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15581	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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	0.55	5/2958 (0.2%)	0.49	7/4002 (0.2%)
1	B	0.13	0/2910	0.30	0/3937
1	E	0.10	0/2920	0.30	0/3951
1	F	0.11	0/2914	0.33	0/3943
2	D	0.18	0/1317	0.48	0/1783
2	Y	0.49	3/1429 (0.2%)	0.63	2/1933 (0.1%)
2	Z	0.68	6/1368 (0.4%)	0.75	11/1854 (0.6%)
All	All	0.36	14/15816 (0.1%)	0.45	20/21403 (0.1%)

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	F	0	1
2	D	0	2
2	Y	0	3
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	ARG	C-O	20.91	1.48	1.23
2	Z	519	LEU	CA-C	-15.24	1.33	1.52
2	Y	518	HIS	CA-C	-13.50	1.35	1.53
1	A	176	HIS	N-CA	-11.20	1.31	1.46
1	A	176	HIS	CA-C	-8.49	1.41	1.52
1	A	176	HIS	C-O	-8.37	1.12	1.23
2	Z	519	LEU	CA-CB	-8.13	1.37	1.54
2	Z	519	LEU	C-O	-8.12	1.13	1.23
2	Z	520	LEU	CA-CB	-7.41	1.43	1.53
1	A	176	HIS	CA-CB	-7.08	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	518	HIS	C-O	-6.38	1.15	1.24
2	Z	519	LEU	C-N	-6.22	1.25	1.33
2	Y	518	HIS	CA-CB	-5.93	1.43	1.53
2	Z	516	SER	N-CA	5.34	1.52	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	519	LEU	CA-C-N	-10.53	102.54	121.81
2	Z	519	LEU	C-N-CA	-10.53	102.54	121.81
1	A	-5	PRO	N-CA-CB	7.95	110.39	103.31
1	A	176	HIS	CA-C-N	-7.37	109.86	123.05
1	A	176	HIS	C-N-CA	-7.37	109.86	123.05
1	A	367	ILE	CB-CA-C	-7.26	97.08	111.60
2	Z	630	PRO	N-CA-CB	6.88	110.48	103.25
2	Z	519	LEU	CB-CA-C	-6.81	95.84	109.79
2	Z	519	LEU	N-CA-CB	-6.74	99.83	111.55
1	A	176	HIS	N-CA-CB	-6.66	101.74	110.59
2	Y	517	GLN	O-C-N	-6.40	116.18	123.48
2	Z	519	LEU	O-C-N	-6.36	114.88	123.15
2	Y	518	HIS	CB-CA-C	-6.29	100.99	113.45
2	Z	515	GLN	CA-C-N	-5.87	113.60	122.81
2	Z	515	GLN	C-N-CA	-5.87	113.60	122.81
2	Z	520	LEU	O-C-N	5.69	128.87	122.32
1	A	366	ARG	CA-C-O	5.68	126.97	120.84
2	Z	516	SER	N-CA-C	5.40	118.36	109.72
1	A	365	MET	O-C-N	5.40	129.13	123.03
2	Z	518	HIS	O-C-N	-5.39	116.07	122.65

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	612	ARG	Peptide
2	D	642	TRP	Peptide
1	F	280	ARG	Peptide
2	Y	517	GLN	Mainchain
2	Y	522	PRO	Peptide
2	Y	526	ALA	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	2912	0	2944	65	0
1	B	2865	0	2913	49	0
1	E	2874	0	2921	34	0
1	F	2869	0	2916	42	0
2	D	1300	0	1283	54	0
2	Y	1409	0	1411	71	0
2	Z	1352	0	1318	38	0
All	All	15581	0	15706	315	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 10.

All (315) 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)
2:Y:609:ARG:HD3	2:D:524:THR:HB	1.54	0.90
1:A:367:ILE:OXT	1:A:367:ILE:HG22	1.73	0.88
1:B:241:LYS:HZ1	2:D:612:ARG:HG3	1.39	0.86
1:B:343:ASP:OD1	1:B:346:ARG:HD2	1.79	0.83
1:B:241:LYS:NZ	2:D:612:ARG:HG3	1.97	0.78
1:B:363:MET:HG3	2:Y:520:LEU:CD1	2.13	0.78
1:A:283:ARG:HG3	1:A:367:ILE:HD12	1.67	0.76
1:B:363:MET:HG3	2:Y:520:LEU:HD13	1.67	0.75
1:A:248:VAL:HG13	2:Z:520:LEU:HD21	1.68	0.74
1:A:41:GLY:HA2	1:A:62:GLY:HA2	1.70	0.74
2:Y:556:THR:HG21	2:D:610:ALA:HB2	1.68	0.74
2:D:474:LEU:HB2	2:D:478:TYR:HB2	1.68	0.74
2:Z:487:LEU:HD23	2:Z:645:LEU:O	1.87	0.73
2:Y:652:THR:HG22	2:Z:643:VAL:HG11	1.70	0.72
1:A:150:GLN:O	1:A:150:GLN:HG2	1.88	0.72
2:D:600:ALA:HA	2:D:603:SER:HB3	1.71	0.71
2:Y:475:LEU:HD11	2:Z:647:LEU:HD13	1.72	0.70
2:Y:569:SER:OG	2:Y:609:ARG:NH1	2.19	0.70
2:Y:634:GLN:HG3	2:Y:638:GLY:HA2	1.75	0.69
1:E:152:ILE:HD11	2:Y:467:LEU:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:487:LEU:HG	2:D:645:LEU:HD22	1.76	0.67
2:D:525:PHE:HZ	2:D:559:VAL:HG13	1.59	0.67
2:Z:548:GLU:HB2	2:Z:561:ALA:HB3	1.76	0.67
1:A:66:PHE:HB2	1:F:152:ILE:HG12	1.77	0.66
1:B:46:LEU:HD13	1:B:55:ASP:HB3	1.78	0.66
2:D:616:LEU:HA	2:D:619:MET:HB2	1.78	0.66
2:Y:599:LEU:HD12	2:Y:601:THR:H	1.60	0.66
1:A:248:VAL:HG13	2:Z:520:LEU:CD2	2.27	0.65
1:F:280:ARG:NH1	1:F:322:ILE:HB	2.12	0.65
2:Z:477:ILE:HD11	2:Z:489:LEU:HD12	1.79	0.65
2:Z:493:HIS:HA	2:Z:496:ALA:HB3	1.78	0.65
1:A:163:VAL:O	1:A:191:ARG:HA	1.97	0.64
2:D:525:PHE:CZ	2:D:559:VAL:HG13	2.33	0.64
2:Y:600:ALA:HA	2:Y:603:SER:HB3	1.78	0.64
2:Y:566:LEU:HD23	2:Y:605:HIS:HB3	1.79	0.63
1:A:54:ILE:HG23	1:A:233:ILE:HG12	1.80	0.63
1:B:14:PRO:HB2	1:B:45:LEU:HD12	1.81	0.63
1:E:145:TYR:O	1:E:177:ARG:NH2	2.32	0.63
1:A:286:LEU:O	1:A:315:GLU:HA	1.99	0.63
1:B:261:ARG:HB2	1:B:337:MET:HG3	1.81	0.62
1:B:150:GLN:OE1	2:Y:612:ARG:NH1	2.31	0.62
1:F:159:LEU:HD21	1:F:170:LEU:HB3	1.82	0.62
1:A:127:ALA:HB1	1:A:189:LEU:HD13	1.83	0.61
1:B:143:VAL:HG23	1:B:159:LEU:HD11	1.82	0.61
1:A:148:ALA:HB2	1:A:174:ASP:HA	1.83	0.61
1:F:259:LEU:HD11	1:F:264:LEU:HD22	1.80	0.61
2:D:479:ILE:HG23	2:D:490:ILE:HB	1.83	0.61
2:Y:615:THR:O	2:Y:616:LEU:HB2	1.99	0.60
2:D:488:LEU:HD13	2:D:643:VAL:HG22	1.83	0.60
1:A:36:ILE:HD12	1:A:68:ILE:HD11	1.84	0.60
2:D:527:ALA:HB3	2:D:556:THR:HA	1.84	0.59
2:D:622:LEU:HD23	2:D:622:LEU:O	2.02	0.59
1:F:268:LEU:HB3	1:F:322:ILE:HD11	1.84	0.59
2:Y:488:LEU:HB3	2:Y:643:VAL:HG22	1.85	0.59
1:E:350:PHE:HB2	1:E:360:TYR:HB3	1.84	0.59
1:F:255:LYS:HB2	1:F:341:PHE:HB2	1.83	0.59
1:E:28:LEU:HG	2:Y:510:GLU:HG3	1.85	0.59
1:A:145:TYR:O	1:A:177:ARG:NH2	2.36	0.59
1:F:311:TYR:OH	1:F:313:GLY:O	2.12	0.59
1:F:15:LEU:HD11	1:F:75:PHE:CD2	2.39	0.58
2:D:479:ILE:HD11	2:D:619:MET:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG22	1:F:152:ILE:HG13	1.86	0.58
2:Z:600:ALA:O	2:Z:603:SER:OG	2.20	0.58
2:Y:632:SER:HB3	2:Y:642:TRP:HH2	1.69	0.58
2:Y:552:MET:HB2	2:Y:556:THR:HG23	1.85	0.58
1:A:248:VAL:HG13	2:Z:520:LEU:HD11	1.86	0.57
1:E:286:LEU:O	1:E:315:GLU:HA	2.05	0.57
2:D:535:LEU:HD12	2:D:557:LEU:HD13	1.85	0.57
1:A:300:GLN:O	1:B:96:ARG:NH2	2.37	0.57
2:Y:496:ALA:HA	2:Y:499:VAL:HG12	1.88	0.56
2:Y:474:LEU:HG	2:Y:480:LEU:HD22	1.87	0.56
2:Z:474:LEU:HG	2:Z:475:LEU:H	1.71	0.56
1:F:127:ALA:HB1	1:F:189:LEU:HD13	1.87	0.56
2:Y:520:LEU:HB3	2:Y:521:ILE:HG13	1.88	0.56
2:Y:527:ALA:HB3	2:Y:556:THR:HA	1.87	0.55
2:D:542:LEU:HD13	2:D:549:LEU:HD21	1.89	0.55
1:F:156:LEU:HD22	1:F:173:THR:HG23	1.89	0.55
1:E:127:ALA:HB1	1:E:189:LEU:HD13	1.88	0.55
1:E:152:ILE:CD1	2:Y:467:LEU:HB2	2.36	0.55
2:Y:639:ARG:NH2	2:Z:651:ASP:OD1	2.40	0.55
2:D:496:ALA:HA	2:D:499:VAL:HG12	1.89	0.54
2:Z:566:LEU:HD13	2:Z:574:LEU:HD22	1.88	0.54
1:A:15:LEU:HD11	1:A:75:PHE:CD2	2.43	0.54
2:D:566:LEU:HD22	2:D:574:LEU:HD21	1.88	0.54
1:B:145:TYR:O	1:B:177:ARG:NH2	2.41	0.54
2:Y:479:ILE:HG23	2:Y:490:ILE:HB	1.89	0.54
2:D:514:LEU:HD13	2:D:545:PHE:HA	1.90	0.54
2:Z:487:LEU:HD21	2:Z:645:LEU:HD22	1.90	0.54
1:E:163:VAL:O	1:E:191:ARG:HA	2.08	0.54
2:Y:477:ILE:HD13	2:D:553:GLY:HA3	1.89	0.53
2:Y:581:GLU:HG2	2:Y:597:ARG:HG3	1.91	0.53
1:F:280:ARG:HB3	1:F:280:ARG:CZ	2.39	0.53
2:D:625:ASP:OD1	2:D:626:MET:N	2.41	0.53
2:D:486:SER:HB2	2:D:645:LEU:HD23	1.89	0.52
2:Y:609:ARG:HD3	2:D:524:THR:CB	2.35	0.52
2:Y:487:LEU:HD23	2:Z:474:LEU:HD22	1.90	0.52
1:A:52:ILE:HD12	1:A:199:LYS:HD3	1.91	0.52
2:D:599:LEU:HD12	2:D:601:THR:H	1.74	0.52
1:A:162:GLN:HE22	1:A:191:ARG:HH21	1.56	0.52
1:A:275:ALA:HB2	1:A:295:CYS:HB3	1.91	0.52
1:B:159:LEU:HD21	1:B:170:LEU:HB3	1.92	0.52
1:A:8:ARG:HD3	1:A:83:PRO:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:522:PRO:HB3	2:D:559:VAL:O	2.09	0.51
2:D:599:LEU:O	2:D:602:MET:N	2.43	0.51
1:B:139:MET:O	1:B:143:VAL:HG22	2.10	0.51
1:A:21:ILE:HD13	1:A:54:ILE:HG13	1.91	0.51
2:Z:492:MET:HG3	2:Z:493:HIS:CD2	2.45	0.51
1:B:121:VAL:HG22	1:B:234:VAL:HG11	1.93	0.51
1:F:272:SER:HB3	1:F:322:ILE:HD13	1.93	0.51
2:Y:614:LEU:HD22	2:Y:618:GLU:HG3	1.92	0.51
2:Z:524:THR:HG22	2:Z:558:ALA:HB2	1.92	0.51
2:Y:547:LEU:HG	2:Y:563:PRO:HD3	1.90	0.51
2:D:639:ARG:HG3	2:D:640:PRO:HD2	1.91	0.51
1:E:90:LEU:HB3	1:E:97:LEU:HD11	1.92	0.50
2:D:625:ASP:O	2:D:629:THR:OG1	2.28	0.50
1:A:156:LEU:HD22	1:A:173:THR:HG23	1.92	0.50
1:F:338:GLN:HB2	1:F:353:PRO:HG3	1.93	0.50
2:Y:480:LEU:HA	2:Y:488:LEU:O	2.10	0.50
2:Y:650:LEU:HA	2:Y:653:LEU:HD13	1.93	0.50
2:Y:477:ILE:HD11	2:Z:647:LEU:HD11	1.94	0.50
2:Z:529:HIS:CE1	2:Z:531:GLU:HA	2.46	0.50
2:Y:535:LEU:HD11	2:Y:549:LEU:HG	1.92	0.50
1:A:248:VAL:HG13	2:Z:520:LEU:CD1	2.42	0.50
1:A:3:ILE:HG12	1:A:90:LEU:O	2.12	0.50
1:B:350:PHE:HB2	1:B:360:TYR:HB3	1.93	0.49
2:Y:620:ASN:HA	2:Y:623:LEU:HB2	1.93	0.49
1:B:15:LEU:HD11	1:B:75:PHE:CD2	2.47	0.49
2:Y:494:ALA:O	2:Y:498:ARG:HG2	2.12	0.49
1:A:15:LEU:HD12	1:A:79:LEU:HD12	1.93	0.49
1:F:21:ILE:HD13	1:F:54:ILE:HG13	1.94	0.49
2:Y:607:SER:OG	2:Y:608:ILE:N	2.46	0.49
1:A:139:MET:HE2	1:A:170:LEU:HG	1.95	0.49
2:Y:598:ILE:HA	2:Y:602:MET:HB3	1.95	0.49
1:E:139:MET:O	1:E:143:VAL:HG22	2.12	0.49
2:Y:636:ASN:HD22	2:D:529:HIS:CE1	2.31	0.49
2:D:619:MET:O	2:D:623:LEU:HD23	2.12	0.49
2:Y:504:MET:HB3	2:Y:598:ILE:HD11	1.95	0.49
1:A:156:LEU:HD13	1:A:174:ASP:O	2.13	0.48
1:B:21:ILE:HG23	1:B:203:GLU:HG3	1.95	0.48
2:Y:471:ILE:HD13	2:Y:482:GLN:HB2	1.95	0.48
2:D:520:LEU:HD12	2:D:520:LEU:H	1.79	0.48
1:A:21:ILE:HA	1:A:199:LYS:HE2	1.96	0.48
1:F:69:THR:OG1	1:F:111:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLY:HA3	1:A:196:LEU:O	2.14	0.48
1:E:75:PHE:HE1	1:E:99:LEU:HD21	1.79	0.48
1:E:96:ARG:NH2	1:F:300:GLN:O	2.45	0.48
2:Y:523:VAL:HG22	2:Y:559:VAL:H	1.78	0.48
1:A:150:GLN:O	1:A:150:GLN:CG	2.61	0.48
1:B:38:GLY:O	1:B:65:ASP:HA	2.14	0.48
1:F:14:PRO:HB2	1:F:45:LEU:HD12	1.95	0.48
1:E:272:SER:HB3	1:E:322:ILE:HD13	1.95	0.47
2:Y:609:ARG:CD	2:D:524:THR:HB	2.35	0.47
2:D:488:LEU:HD22	2:D:643:VAL:HG13	1.95	0.47
1:A:365:MET:HB3	2:Z:517:GLN:OE1	2.15	0.47
1:F:28:LEU:HB2	1:F:31:LEU:HD12	1.95	0.47
1:A:248:VAL:HG22	2:Z:520:LEU:HD22	1.95	0.47
1:F:144:GLN:HG3	1:F:145:TYR:N	2.30	0.47
1:F:322:ILE:HG23	1:F:326:MET:HE2	1.96	0.47
2:Y:468:GLY:HA2	2:Y:483:ALA:HB2	1.96	0.47
1:B:92:TRP:NE1	1:B:94:ASP:O	2.48	0.47
1:B:291:LEU:HB2	1:B:309:ILE:HD13	1.96	0.47
1:E:363:MET:HG3	1:E:364:PRO:HD2	1.96	0.47
2:Y:551:ASP:HA	2:Y:557:LEU:HD23	1.96	0.47
1:B:69:THR:HG1	1:B:111:LEU:HB2	1.79	0.47
2:Y:553:GLY:O	2:Y:556:THR:HG22	2.14	0.47
2:Y:604:CYS:SG	2:D:576:ARG:NH1	2.88	0.47
1:A:215:ILE:HD11	1:A:226:PHE:HB3	1.97	0.46
1:E:136:PHE:HE2	1:E:204:LEU:HD21	1.79	0.46
2:D:524:THR:HG22	2:D:556:THR:OG1	2.15	0.46
1:B:69:THR:OG1	1:B:111:LEU:HB2	2.14	0.46
1:F:98:THR:HG21	1:F:100:LYS:HE3	1.96	0.46
2:Y:479:ILE:HD11	2:Y:619:MET:HB3	1.97	0.46
2:Z:569:SER:OG	2:Z:570:ASP:N	2.48	0.46
1:A:18:PHE:HE2	1:A:45:LEU:HB2	1.81	0.46
2:Y:609:ARG:HG3	2:Y:610:ALA:H	1.80	0.46
1:A:99:LEU:HB2	1:A:106:PHE:HB2	1.97	0.46
2:Z:618:GLU:HA	2:Z:621:ALA:HB3	1.97	0.46
1:B:215:ILE:HD11	1:B:226:PHE:HB3	1.96	0.46
1:E:18:PHE:CE2	1:E:45:LEU:HB2	2.50	0.46
1:F:290:LEU:HD11	1:F:306:GLU:HB3	1.97	0.46
1:E:280:ARG:HH22	1:E:326:MET:HE1	1.81	0.46
1:A:-3:GLY:HA2	1:A:93:ASP:OD1	2.16	0.46
2:Z:501:TYR:O	2:Z:504:MET:HB2	2.16	0.46
1:B:4:LEU:HD23	1:B:90:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ARG:HH12	1:F:322:ILE:HB	1.81	0.46
2:Y:605:HIS:ND1	2:Y:606:GLY:O	2.49	0.46
1:F:8:ARG:HD3	1:F:83:PRO:O	2.16	0.45
2:Y:474:LEU:HD12	2:Y:480:LEU:HB3	1.97	0.45
2:Y:648:LYS:HA	2:Y:648:LYS:HD3	1.82	0.45
2:Z:521:ILE:O	2:Z:521:ILE:HG13	2.16	0.45
1:F:8:ARG:HD2	1:F:79:LEU:O	2.16	0.45
2:D:481:ALA:O	2:D:487:LEU:HA	2.17	0.45
1:A:178:LEU:HD13	1:A:248:VAL:HG11	1.97	0.45
1:B:148:ALA:HB2	1:B:174:ASP:HA	1.99	0.45
1:B:268:LEU:HD22	1:B:322:ILE:HG13	1.99	0.45
2:D:627:GLU:OE1	2:D:627:GLU:N	2.48	0.45
1:E:18:PHE:CZ	1:E:56:THR:HG22	2.51	0.45
2:Z:612:ARG:HD3	2:Z:612:ARG:HA	1.78	0.45
1:B:54:ILE:HG23	1:B:233:ILE:HG12	1.99	0.45
1:F:155:TYR:HA	1:F:238:ILE:HG21	1.99	0.45
1:F:268:LEU:HD23	1:F:293:VAL:HG11	1.97	0.45
1:A:18:PHE:HE1	1:A:54:ILE:HG22	1.80	0.45
2:Y:603:SER:C	2:Y:605:HIS:H	2.26	0.44
1:A:139:MET:O	1:A:143:VAL:HG22	2.18	0.44
2:Z:472:ALA:H	2:Z:479:ILE:HG23	1.81	0.44
1:E:69:THR:OG1	1:E:111:LEU:HB2	2.17	0.44
1:E:99:LEU:HB2	1:E:106:PHE:HB2	2.00	0.44
1:F:352:VAL:HB	1:F:355:ASN:HB3	1.99	0.44
1:A:36:ILE:HG12	1:A:45:LEU:HD22	2.00	0.44
1:F:139:MET:O	1:F:143:VAL:HG22	2.17	0.44
2:D:581:GLU:HG2	2:D:597:ARG:HG2	1.99	0.44
1:A:35:LEU:HD12	1:A:68:ILE:O	2.17	0.44
1:A:159:LEU:HD21	1:A:170:LEU:HB3	2.00	0.44
1:B:340:ALA:HB3	1:B:349:LEU:HB3	1.98	0.44
2:Z:474:LEU:HD21	2:Z:477:ILE:HG23	2.00	0.44
2:D:612:ARG:NH2	2:D:614:LEU:HD11	2.32	0.44
1:A:8:ARG:HD2	1:A:79:LEU:O	2.18	0.44
1:B:5:GLN:HG2	1:B:87:LEU:HD11	2.00	0.44
1:E:35:LEU:HD12	1:E:68:ILE:O	2.17	0.44
2:Y:570:ASP:O	2:Y:570:ASP:CG	2.61	0.44
1:B:284:LEU:HD23	1:B:320:PHE:HD2	1.83	0.44
1:E:261:ARG:NH1	1:E:329:LEU:O	2.49	0.44
1:B:352:VAL:HB	1:B:355:ASN:HB3	2.00	0.44
1:E:21:ILE:HA	1:E:199:LYS:HE2	1.99	0.44
2:Y:471:ILE:HG13	2:Y:480:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HG	1:A:59:PRO:HG3	1.99	0.43
1:E:54:ILE:HG23	1:E:233:ILE:HG12	2.00	0.43
2:D:470:ALA:HA	2:D:481:ALA:HA	2.00	0.43
2:Y:646:THR:HG23	2:Y:648:LYS:H	1.83	0.43
1:B:94:ASP:HB3	1:B:95:ASN:H	1.58	0.43
1:E:91:ASP:O	1:E:97:LEU:HD12	2.18	0.43
1:F:38:GLY:HA3	1:F:66:PHE:CE1	2.53	0.43
2:Y:508:ARG:HD3	2:Y:514:LEU:HD12	1.99	0.43
1:A:158:GLY:CA	1:A:196:LEU:O	2.66	0.43
1:E:297:ASN:HD21	1:E:301:GLU:HB2	1.82	0.43
2:D:566:LEU:HA	2:D:605:HIS:CE1	2.53	0.43
1:A:177:ARG:HD3	1:A:324:TYR:CD1	2.53	0.43
2:Y:538:HIS:O	2:Y:538:HIS:ND1	2.52	0.43
1:A:174:ASP:OD1	1:A:177:ARG:HG2	2.18	0.43
1:E:21:ILE:HG23	1:E:203:GLU:HG3	2.00	0.43
1:B:139:MET:HE2	1:B:170:LEU:HG	2.00	0.43
1:B:151:ASP:OD1	1:B:152:ILE:N	2.52	0.43
1:E:18:PHE:O	1:E:22:VAL:HG23	2.18	0.43
1:A:18:PHE:CE2	1:A:56:THR:HG22	2.54	0.43
1:A:82:LEU:HD23	1:B:270:ARG:HD3	2.01	0.43
1:B:136:PHE:HE2	1:B:204:LEU:HD21	1.84	0.43
1:F:160:LEU:HD11	1:F:193:GLU:HB2	2.01	0.43
2:Y:493:HIS:ND1	2:D:555:ASN:OD1	2.52	0.43
1:A:-4:ARG:HA	1:F:176:HIS:CE1	2.54	0.42
1:B:339:LEU:HB3	1:B:341:PHE:HE1	1.83	0.42
2:Y:547:LEU:HD13	2:Y:575:ALA:HA	2.00	0.42
2:D:569:SER:HB3	2:D:605:HIS:CD2	2.54	0.42
1:A:14:PRO:HB2	1:A:45:LEU:HD12	2.00	0.42
1:E:30:ILE:HG12	1:E:116:PHE:HD1	1.85	0.42
2:Y:570:ASP:OD1	2:Y:573:SER:OG	2.33	0.42
2:D:646:THR:O	2:D:646:THR:OG1	2.36	0.42
1:A:248:VAL:CG1	2:Z:520:LEU:HD11	2.49	0.42
2:Y:653:LEU:O	2:Z:640:PRO:HD2	2.19	0.42
1:A:164:GLU:OE1	1:A:169:ARG:NH2	2.45	0.42
1:A:268:LEU:HD23	1:A:293:VAL:HG11	2.02	0.42
1:A:128:THR:HG23	1:A:218:GLU:HG2	2.01	0.42
1:F:136:PHE:HE2	1:F:204:LEU:HD21	1.83	0.42
2:Z:487:LEU:HD22	2:Z:650:LEU:HD11	2.01	0.42
2:D:564:VAL:HG23	2:D:565:MET:HG3	2.01	0.42
2:D:612:ARG:O	2:D:613:ARG:C	2.63	0.42
1:E:15:LEU:HD11	1:E:75:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:566:LEU:HD22	2:Y:574:LEU:HD21	2.01	0.42
2:D:535:LEU:HD13	2:D:557:LEU:HD22	2.02	0.42
2:D:608:ILE:HG21	2:D:612:ARG:HD3	2.01	0.42
1:B:255:LYS:HB2	1:B:341:PHE:HB2	2.02	0.42
2:Z:473:GLN:HA	2:Z:478:TYR:HA	2.02	0.42
1:B:35:LEU:HD12	1:B:68:ILE:O	2.20	0.42
1:F:215:ILE:HA	1:F:228:CYS:HB3	2.02	0.42
2:Z:530:GLU:HG2	2:Z:532:CYS:SG	2.60	0.42
2:D:490:ILE:HA	2:D:641:THR:O	2.20	0.42
1:A:92:TRP:CD2	1:F:152:ILE:HB	2.54	0.42
1:B:144:GLN:HG3	1:B:145:TYR:N	2.34	0.42
1:E:198:ARG:O	1:E:202:LEU:HG	2.19	0.42
2:Y:625:ASP:OD1	2:Y:626:MET:N	2.51	0.42
1:F:195:ILE:HG22	1:F:238:ILE:HD12	2.01	0.41
2:Y:501:TYR:CD1	2:Y:599:LEU:HA	2.55	0.41
1:A:273:ILE:HG21	1:B:78:ILE:HG13	2.02	0.41
2:Y:620:ASN:O	2:Y:624:ARG:HG2	2.20	0.41
1:A:38:GLY:HA3	1:A:66:PHE:CE2	2.55	0.41
1:F:15:LEU:HD12	1:F:79:LEU:HD12	2.00	0.41
1:F:318:VAL:HG11	1:F:341:PHE:HE2	1.85	0.41
2:Z:613:ARG:H	2:Z:613:ARG:HD3	1.85	0.41
1:A:36:ILE:HB	1:A:68:ILE:HG12	2.02	0.41
1:B:160:LEU:HD11	1:B:193:GLU:HB2	2.02	0.41
1:B:286:LEU:O	1:B:315:GLU:HA	2.21	0.41
1:B:178:LEU:HD13	1:B:248:VAL:HG11	2.01	0.41
1:B:156:LEU:HD22	1:B:173:THR:HG23	2.03	0.41
1:E:28:LEU:HD23	1:E:28:LEU:HA	1.91	0.41
2:D:480:LEU:HD12	2:D:487:LEU:HD13	2.02	0.41
2:D:480:LEU:HA	2:D:488:LEU:O	2.21	0.41
1:B:35:LEU:HD23	1:B:46:LEU:HD23	2.03	0.41
1:E:159:LEU:HD21	1:E:170:LEU:HD22	2.02	0.41
2:Z:581:GLU:HG3	2:Z:598:ILE:HD13	2.02	0.41
1:B:129:PHE:CE1	1:B:163:VAL:HG11	2.56	0.40
1:F:318:VAL:HG11	1:F:341:PHE:CE2	2.56	0.40
2:Z:519:LEU:HD13	2:Z:560:ARG:C	2.45	0.40
2:D:501:TYR:CZ	2:D:505:LYS:HD2	2.56	0.40
1:A:274:LEU:HB2	1:A:303:ALA:HB2	2.03	0.40
2:Y:472:ALA:HB3	2:Z:471:ILE:HG23	2.03	0.40
2:D:564:VAL:C	2:D:566:LEU:H	2.28	0.40
1:A:350:PHE:HB2	1:A:360:TYR:HB3	2.02	0.40
1:F:286:LEU:O	1:F:315:GLU:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:474:LEU:HB2	2:Y:478:TYR:HB2	2.03	0.40
2:Y:474:LEU:O	2:Y:475:LEU:HG	2.22	0.40
1:A:347:SER:HB3	1:A:361:ILE:HG23	2.04	0.40
2:Y:488:LEU:HD22	2:Y:643:VAL:CG1	2.51	0.40
1:A:13:LYS:HB3	1:A:14:PRO:HD3	2.02	0.40
1:B:220:LEU:HB2	1:B:223:GLN:HB2	2.04	0.40
1:E:347:SER:HB3	1:E:361:ILE:HG23	2.03	0.40
1:F:198:ARG:O	1:F:202:LEU:HG	2.22	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	372/387 (96%)	357 (96%)	15 (4%)	0	100	100
1	B	364/387 (94%)	352 (97%)	12 (3%)	0	100	100
1	E	365/387 (94%)	354 (97%)	11 (3%)	0	100	100
1	F	365/387 (94%)	352 (96%)	13 (4%)	0	100	100
2	D	170/220 (77%)	137 (81%)	32 (19%)	1 (1%)	21	54
2	Y	182/220 (83%)	132 (72%)	48 (26%)	2 (1%)	11	43
2	Z	183/220 (83%)	145 (79%)	37 (20%)	1 (0%)	24	57
All	All	2001/2208 (91%)	1829 (91%)	168 (8%)	4 (0%)	43	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	616	LEU
2	D	526	ALA
2	Y	612	ARG

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Mol	Chain	Res	Type
2	Z	629	THR

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	313/329 (95%)	313 (100%)	0	100	100
1	B	311/329 (94%)	310 (100%)	1 (0%)	86	83
1	E	312/329 (95%)	312 (100%)	0	100	100
1	F	311/329 (94%)	311 (100%)	0	100	100
2	D	131/180 (73%)	131 (100%)	0	100	100
2	Y	148/180 (82%)	148 (100%)	0	100	100
2	Z	131/180 (73%)	131 (100%)	0	100	100
All	All	1657/1856 (89%)	1656 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	346	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	133	GLN
1	A	229	ASN
1	A	287	GLN
1	A	345	ASN
1	B	5	GLN
1	B	246	ASN
1	E	5	GLN
1	E	109	GLN

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Mol	Chain	Res	Type
1	E	133	GLN
1	E	210	ASN
1	E	229	ASN
1	E	287	GLN
1	E	298	ASN
1	F	276	ASN
1	F	298	ASN
2	Y	515	GLN
2	Y	636	ASN
2	Z	493	HIS
2	Z	507	GLN
2	Z	518	HIS
2	Z	529	HIS
2	D	605	HIS
2	D	620	ASN

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

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	374/387 (96%)	0.13	11 (2%) 53 31	67, 103, 130, 146	0
1	B	366/387 (94%)	0.06	2 (0%) 87 68	74, 117, 152, 166	0
1	E	367/387 (94%)	0.13	3 (0%) 82 60	82, 123, 159, 169	0
1	F	367/387 (94%)	0.09	4 (1%) 78 54	71, 97, 125, 142	0
2	D	176/220 (80%)	0.98	24 (13%) 7 5	132, 161, 189, 202	0
2	Y	186/220 (84%)	0.83	23 (12%) 8 6	109, 147, 180, 192	0
2	Z	187/220 (85%)	0.73	13 (6%) 22 14	118, 166, 184, 203	0
All	All	2023/2208 (91%)	0.31	80 (3%) 42 23	67, 121, 173, 203	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	63	ALA	5.1
1	A	20	GLY	3.8
1	A	92	TRP	3.7
2	D	525	PHE	3.7
2	Z	496	ALA	3.5
2	Y	568	LYS	3.5
2	D	652	THR	3.4
2	D	644	LYS	3.4
2	Y	607	SER	3.3
1	E	19	THR	3.3
1	F	280	ARG	3.3
2	Y	585	VAL	3.3
2	Z	608	ILE	3.3
2	Y	567	GLY	3.3
2	D	649	GLU	3.2
2	D	645	LEU	3.2
2	Y	608	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	601	THR	3.1
2	D	521	ILE	3.0
1	A	94	ASP	3.0
2	Z	585	VAL	3.0
2	D	608	ILE	3.0
1	A	93	ASP	3.0
2	D	487	LEU	2.9
2	Z	565	MET	2.9
1	F	64	GLY	2.9
2	Y	614	LEU	2.8
2	Z	606	GLY	2.8
2	Y	645	LEU	2.8
2	D	647	LEU	2.8
2	D	474	LEU	2.7
1	A	95	ASN	2.7
2	Y	653	LEU	2.7
2	Y	522	PRO	2.7
1	E	5	GLN	2.6
2	Z	474	LEU	2.6
2	Y	487	LEU	2.6
1	B	367	ILE	2.6
1	F	281	GLY	2.6
1	A	25	LEU	2.5
1	A	19	THR	2.5
2	Y	467	LEU	2.5
2	Y	643	VAL	2.5
2	Y	565	MET	2.4
2	D	628	ASN	2.4
2	Y	586	GLY	2.4
2	Y	523	VAL	2.4
2	D	602	MET	2.4
2	Y	622	LEU	2.4
2	Z	467	LEU	2.3
1	A	144	GLN	2.3
2	Z	653	LEU	2.3
2	D	527	ALA	2.3
2	Y	527	ALA	2.3
2	D	469	PHE	2.3
2	Y	485	ASP	2.3
2	D	565	MET	2.3
2	D	622	LEU	2.2
1	E	95	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	583	ALA	2.2
1	A	64	GLY	2.2
2	Z	643	VAL	2.2
2	D	638	GLY	2.2
2	Y	524	THR	2.2
2	D	473	GLN	2.2
2	Y	555	ASN	2.2
2	D	467	LEU	2.2
2	Y	521	ILE	2.2
2	Y	618	GLU	2.1
2	Y	525	PHE	2.1
1	B	17	ALA	2.1
2	Z	490	ILE	2.1
2	Z	464	LEU	2.1
1	A	203	GLU	2.1
2	Z	477	ILE	2.1
1	A	91	ASP	2.0
2	Z	644	LYS	2.0
2	D	528	SER	2.0
2	D	648	LYS	2.0
2	D	465	PRO	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 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.