



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:11 PM EDT

PDB ID : 4ZC0 / pdb_00004zc0
Title : Structure of a dodecameric bacterial helicase
Authors : Bazin, A.; Cherrier, M.V.; Gutsche, I.; Timmins, J.; Terradot, L.
Deposited on : 2015-04-15
Resolution : 6.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

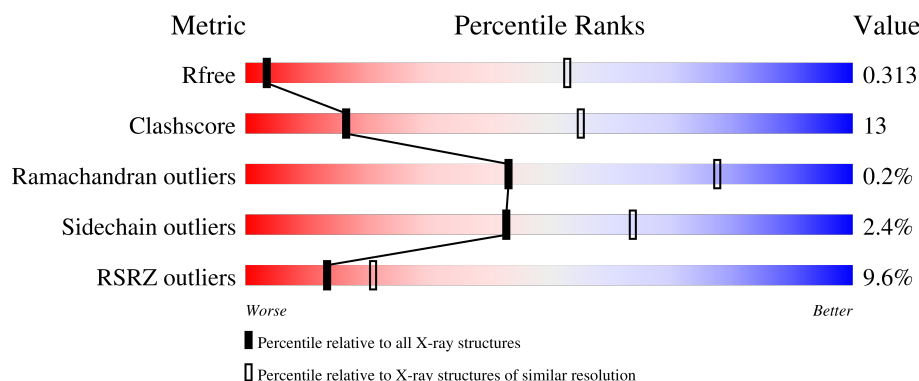
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.70 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	1162 (9.00-4.00)
Clashscore	190562	1001 (9.32-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	521	 9% 59% 26% 15%
1	B	521	 8% 58% 25% 17%
1	C	521	 3% 20% 8% 72%
1	D	521	 2% 19% 8% 72%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TBR	B	501	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9140 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 Replicative DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3491	2199	611	667	14			
1	B	434	Total	C	N	O	S	0	0	0
			3397	2141	595	647	14			
1	C	148	Total	C	N	O	S	0	0	0
			1122	714	193	212	3			
1	D	146	Total	C	N	O	S	0	0	0
			1112	708	191	210	3			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	initiating methionine	UNP O25916
A	-31	HIS	-	expression tag	UNP O25916
A	-30	HIS	-	expression tag	UNP O25916
A	-29	HIS	-	expression tag	UNP O25916
A	-28	HIS	-	expression tag	UNP O25916
A	-27	HIS	-	expression tag	UNP O25916
A	-26	HIS	-	expression tag	UNP O25916
A	-25	GLY	-	expression tag	UNP O25916
A	-24	LYS	-	expression tag	UNP O25916
A	-23	PRO	-	expression tag	UNP O25916
A	-22	ILE	-	expression tag	UNP O25916
A	-21	PRO	-	expression tag	UNP O25916
A	-20	ASN	-	expression tag	UNP O25916
A	-19	PRO	-	expression tag	UNP O25916
A	-18	LEU	-	expression tag	UNP O25916
A	-17	LEU	-	expression tag	UNP O25916
A	-16	GLY	-	expression tag	UNP O25916
A	-15	LEU	-	expression tag	UNP O25916
A	-14	ASP	-	expression tag	UNP O25916
A	-13	SER	-	expression tag	UNP O25916
A	-12	THR	-	expression tag	UNP O25916

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	GLU	-	expression tag	UNP O25916
A	-10	ASN	-	expression tag	UNP O25916
A	-9	LEU	-	expression tag	UNP O25916
A	-8	TYR	-	expression tag	UNP O25916
A	-7	PHE	-	expression tag	UNP O25916
A	-6	GLN	-	expression tag	UNP O25916
A	-5	GLY	-	expression tag	UNP O25916
A	-4	ILE	-	expression tag	UNP O25916
A	-3	ASP	-	expression tag	UNP O25916
A	-2	PRO	-	expression tag	UNP O25916
A	-1	PHE	-	expression tag	UNP O25916
A	0	THR	-	expression tag	UNP O25916
B	-32	MET	-	initiating methionine	UNP O25916
B	-31	HIS	-	expression tag	UNP O25916
B	-30	HIS	-	expression tag	UNP O25916
B	-29	HIS	-	expression tag	UNP O25916
B	-28	HIS	-	expression tag	UNP O25916
B	-27	HIS	-	expression tag	UNP O25916
B	-26	HIS	-	expression tag	UNP O25916
B	-25	GLY	-	expression tag	UNP O25916
B	-24	LYS	-	expression tag	UNP O25916
B	-23	PRO	-	expression tag	UNP O25916
B	-22	ILE	-	expression tag	UNP O25916
B	-21	PRO	-	expression tag	UNP O25916
B	-20	ASN	-	expression tag	UNP O25916
B	-19	PRO	-	expression tag	UNP O25916
B	-18	LEU	-	expression tag	UNP O25916
B	-17	LEU	-	expression tag	UNP O25916
B	-16	GLY	-	expression tag	UNP O25916
B	-15	LEU	-	expression tag	UNP O25916
B	-14	ASP	-	expression tag	UNP O25916
B	-13	SER	-	expression tag	UNP O25916
B	-12	THR	-	expression tag	UNP O25916
B	-11	GLU	-	expression tag	UNP O25916
B	-10	ASN	-	expression tag	UNP O25916
B	-9	LEU	-	expression tag	UNP O25916
B	-8	TYR	-	expression tag	UNP O25916
B	-7	PHE	-	expression tag	UNP O25916
B	-6	GLN	-	expression tag	UNP O25916
B	-5	GLY	-	expression tag	UNP O25916
B	-4	ILE	-	expression tag	UNP O25916
B	-3	ASP	-	expression tag	UNP O25916

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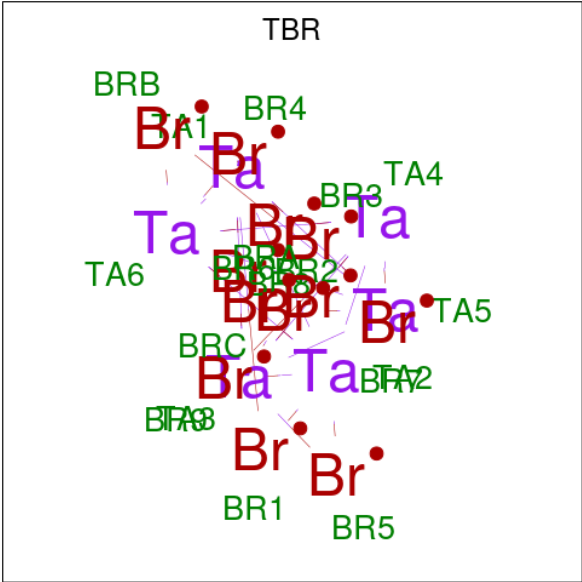
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PRO	-	expression tag	UNP O25916
B	-1	PHE	-	expression tag	UNP O25916
B	0	THR	-	expression tag	UNP O25916
C	-32	MET	-	initiating methionine	UNP O25916
C	-31	HIS	-	expression tag	UNP O25916
C	-30	HIS	-	expression tag	UNP O25916
C	-29	HIS	-	expression tag	UNP O25916
C	-28	HIS	-	expression tag	UNP O25916
C	-27	HIS	-	expression tag	UNP O25916
C	-26	HIS	-	expression tag	UNP O25916
C	-25	GLY	-	expression tag	UNP O25916
C	-24	LYS	-	expression tag	UNP O25916
C	-23	PRO	-	expression tag	UNP O25916
C	-22	ILE	-	expression tag	UNP O25916
C	-21	PRO	-	expression tag	UNP O25916
C	-20	ASN	-	expression tag	UNP O25916
C	-19	PRO	-	expression tag	UNP O25916
C	-18	LEU	-	expression tag	UNP O25916
C	-17	LEU	-	expression tag	UNP O25916
C	-16	GLY	-	expression tag	UNP O25916
C	-15	LEU	-	expression tag	UNP O25916
C	-14	ASP	-	expression tag	UNP O25916
C	-13	SER	-	expression tag	UNP O25916
C	-12	THR	-	expression tag	UNP O25916
C	-11	GLU	-	expression tag	UNP O25916
C	-10	ASN	-	expression tag	UNP O25916
C	-9	LEU	-	expression tag	UNP O25916
C	-8	TYR	-	expression tag	UNP O25916
C	-7	PHE	-	expression tag	UNP O25916
C	-6	GLN	-	expression tag	UNP O25916
C	-5	GLY	-	expression tag	UNP O25916
C	-4	ILE	-	expression tag	UNP O25916
C	-3	ASP	-	expression tag	UNP O25916
C	-2	PRO	-	expression tag	UNP O25916
C	-1	PHE	-	expression tag	UNP O25916
C	0	THR	-	expression tag	UNP O25916
D	-32	MET	-	initiating methionine	UNP O25916
D	-31	HIS	-	expression tag	UNP O25916
D	-30	HIS	-	expression tag	UNP O25916
D	-29	HIS	-	expression tag	UNP O25916
D	-28	HIS	-	expression tag	UNP O25916
D	-27	HIS	-	expression tag	UNP O25916

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-26	HIS	-	expression tag	UNP O25916
D	-25	GLY	-	expression tag	UNP O25916
D	-24	LYS	-	expression tag	UNP O25916
D	-23	PRO	-	expression tag	UNP O25916
D	-22	ILE	-	expression tag	UNP O25916
D	-21	PRO	-	expression tag	UNP O25916
D	-20	ASN	-	expression tag	UNP O25916
D	-19	PRO	-	expression tag	UNP O25916
D	-18	LEU	-	expression tag	UNP O25916
D	-17	LEU	-	expression tag	UNP O25916
D	-16	GLY	-	expression tag	UNP O25916
D	-15	LEU	-	expression tag	UNP O25916
D	-14	ASP	-	expression tag	UNP O25916
D	-13	SER	-	expression tag	UNP O25916
D	-12	THR	-	expression tag	UNP O25916
D	-11	GLU	-	expression tag	UNP O25916
D	-10	ASN	-	expression tag	UNP O25916
D	-9	LEU	-	expression tag	UNP O25916
D	-8	TYR	-	expression tag	UNP O25916
D	-7	PHE	-	expression tag	UNP O25916
D	-6	GLN	-	expression tag	UNP O25916
D	-5	GLY	-	expression tag	UNP O25916
D	-4	ILE	-	expression tag	UNP O25916
D	-3	ASP	-	expression tag	UNP O25916
D	-2	PRO	-	expression tag	UNP O25916
D	-1	PHE	-	expression tag	UNP O25916
D	0	THR	-	expression tag	UNP O25916

- Molecule 2 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).

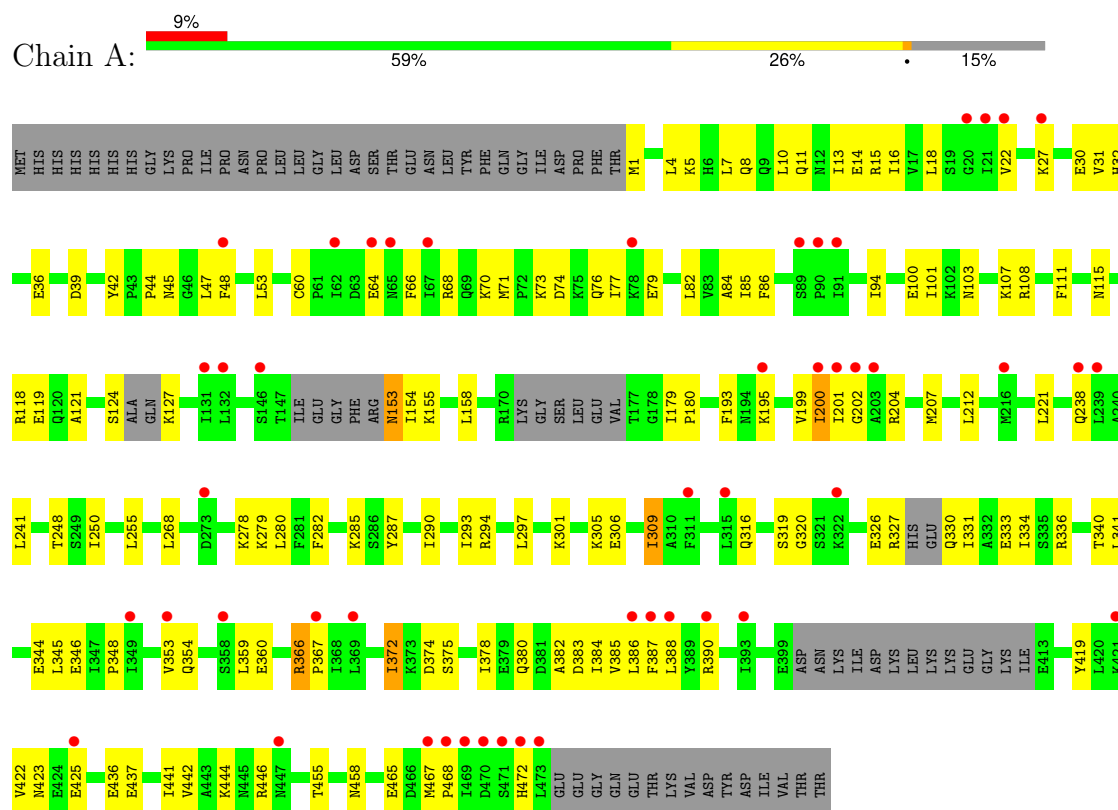


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Br	Ta	0	0
			18	12	6		

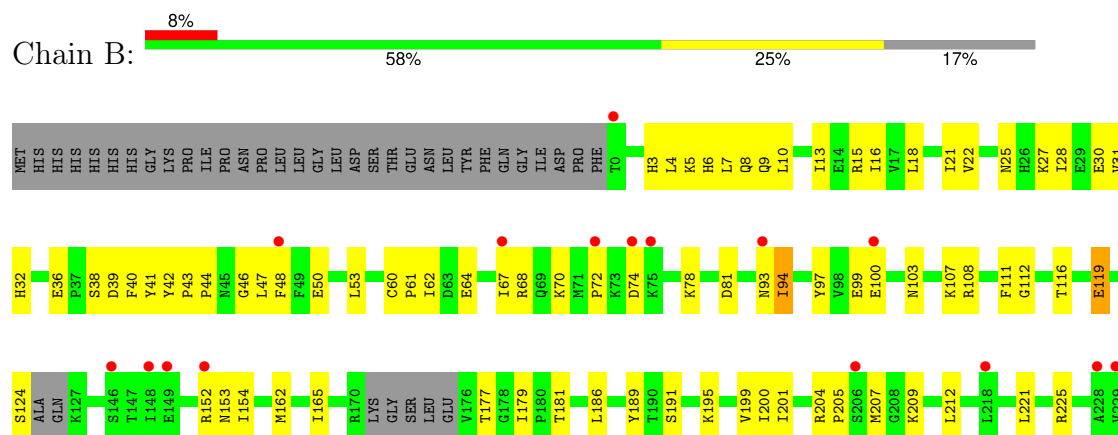
3 Residue-property plots

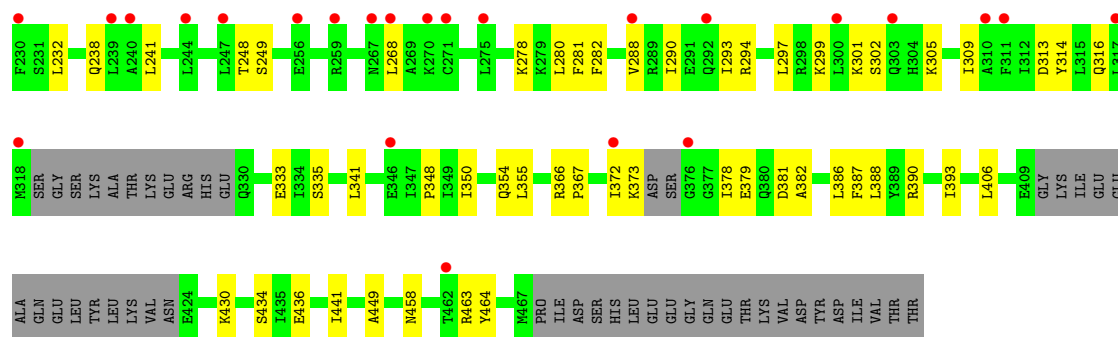
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Replicative DNA helicase

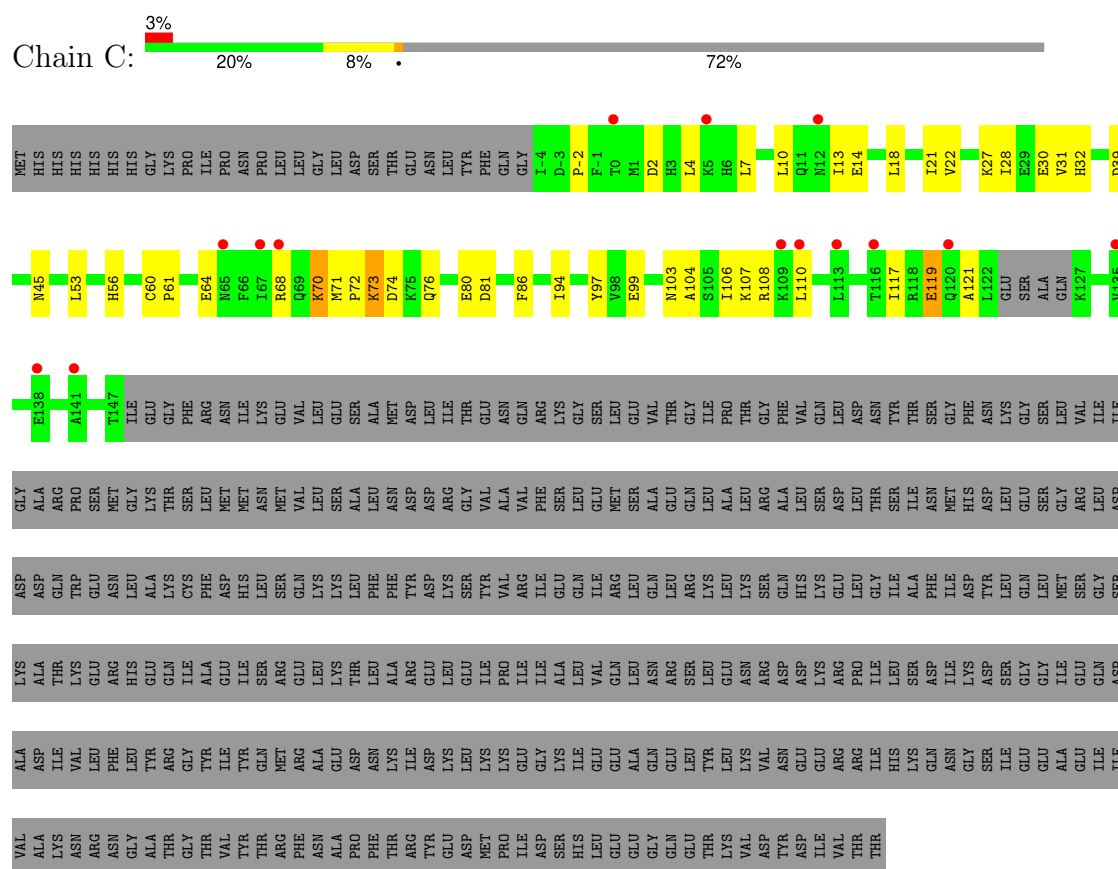


• Molecule 1: Replicative DNA helicase

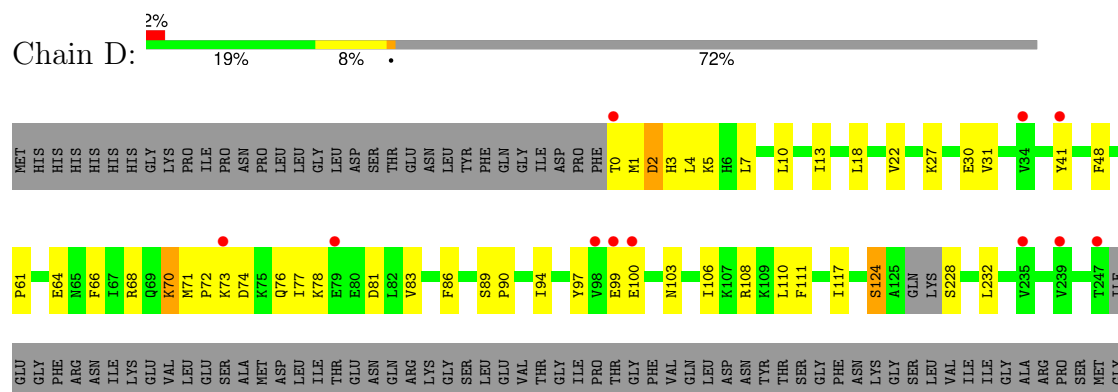




- Molecule 1: Replicative DNA helicase



- Molecule 1: Replicative DNA helicase



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	283.47 Å 283.47 Å 283.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 6.70 47.24 – 6.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.24-6.70) 99.5 (47.24-6.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 6.67 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.258 , 0.299 0.272 , 0.313	Depositor DCC
R_{free} test set	356 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	579.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 477.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	9140	wwPDB-VP
Average B, all atoms (Å ²)	315.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TBR

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	0.32	0/3536	0.82	4/4757 (0.1%)
1	B	0.32	0/3439	0.81	0/4624
1	C	0.36	0/1140	0.90	1/1542 (0.1%)
1	D	0.36	0/1130	0.89	1/1528 (0.1%)
All	All	0.33	0/9245	0.84	6/12451 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-2	PRO	N-CA-CB	8.15	110.13	103.36
1	D	2	ASP	N-CA-C	6.50	118.05	110.97
1	A	74	ASP	N-CA-C	-6.48	105.02	113.12
1	A	366	ARG	CA-C-N	5.55	125.31	119.76
1	A	366	ARG	C-N-CA	5.55	125.31	119.76
1	A	372	ILE	N-CA-C	5.28	111.86	106.21

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	3491	0	3456	97	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3397	0	3357	84	2
1	C	1122	0	1062	30	0
1	D	1112	0	1062	35	0
2	B	18	0	0	6	0
All	All	9140	0	8937	234	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (234) 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:47:LEU:HG	2:B:501:TBR:BR9	2.15	1.01
1:B:301:LYS:NZ	1:B:305:LYS:O	2.07	0.86
1:A:301:LYS:NZ	1:A:305:LYS:O	2.08	0.84
1:C:99:GLU:O	1:C:103:ASN:ND2	2.13	0.81
1:B:39:ASP:O	1:B:108:ARG:NH2	2.14	0.80
1:A:200:ILE:HD12	1:A:382:ALA:HB2	1.66	0.77
1:D:10:LEU:HA	1:D:13:ILE:HD12	1.67	0.76
1:A:330:GLN:N	1:A:333:GLU:OE2	2.20	0.74
1:A:212:LEU:HD13	1:A:388:LEU:HD21	1.73	0.71
1:B:290:ILE:HA	1:B:293:ILE:HD12	1.74	0.70
1:A:73:LYS:HA	1:A:76:GLN:HE22	1.58	0.69
1:A:111:PHE:O	1:A:115:ASN:ND2	2.26	0.69
1:B:355:LEU:HD23	1:B:372:ILE:HB	1.75	0.69
1:D:71:MET:HG2	1:D:76:GLN:HG3	1.75	0.69
1:B:249:SER:HA	1:B:463:ARG:HH22	1.56	0.69
1:A:71:MET:HG2	1:A:76:GLN:HG3	1.74	0.68
1:B:47:LEU:HD21	2:B:501:TBR:BR7	2.48	0.68
1:C:94:ILE:HG13	1:C:97:TYR:HB2	1.74	0.68
1:D:64:GLU:OE1	1:D:68:ARG:NH2	2.27	0.67
1:A:331:ILE:HA	1:A:334:ILE:HB	1.76	0.66
1:A:330:GLN:HA	1:A:330:GLN:HE21	1.61	0.66
1:B:373:LYS:HG2	1:B:378:ILE:HG12	1.77	0.66
1:C:10:LEU:HA	1:C:13:ILE:HD12	1.78	0.65
1:A:195:LYS:HA	1:A:348:PRO:HD3	1.78	0.65
1:A:36:GLU:N	1:A:39:ASP:OD2	2.29	0.65
1:B:13:ILE:HA	1:B:16:ILE:HD12	1.79	0.65
1:C:39:ASP:O	1:C:108:ARG:NH2	2.30	0.65
1:B:212:LEU:HD13	1:B:388:LEU:HD21	1.79	0.64
1:A:124:SER:O	1:A:127:LYS:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:HA	1:A:446:ARG:HE	1.63	0.63
1:C:64:GLU:OE1	1:C:68:ARG:NH2	2.31	0.63
1:A:238:GLN:HA	1:A:241:LEU:HD12	1.79	0.63
1:C:21:ILE:HD11	1:C:31:VAL:HG21	1.79	0.62
1:A:221:LEU:HD22	1:A:278:LYS:HB3	1.82	0.62
1:C:70:LYS:HA	1:C:70:LYS:NZ	2.15	0.62
1:D:1:MET:HG3	1:D:5:LYS:HE3	1.82	0.61
1:A:39:ASP:O	1:A:108:ARG:NH2	2.28	0.61
1:B:36:GLU:N	1:B:39:ASP:OD2	2.32	0.61
1:D:99:GLU:O	1:D:103:ASN:ND2	2.31	0.61
1:D:228:SER:O	1:D:232:LEU:N	2.32	0.61
1:A:14:GLU:OE1	1:A:45:ASN:ND2	2.29	0.61
1:A:11:GLN:HG2	1:A:15:ARG:HE	1.65	0.60
1:A:13:ILE:HA	1:A:16:ILE:HD12	1.84	0.60
1:B:62:ILE:HG23	1:B:67:ILE:HD11	1.84	0.60
1:B:238:GLN:HA	1:B:241:LEU:HD12	1.83	0.60
1:A:387:PHE:HB2	1:A:441:ILE:HB	1.84	0.59
1:B:177:THR:OG1	1:B:191:SER:O	2.19	0.59
1:B:78:LYS:HB2	1:B:81:ASP:OD2	2.03	0.59
1:B:205:PRO:HA	1:B:209:LYS:HE3	1.85	0.59
1:A:290:ILE:HA	1:A:293:ILE:HD12	1.83	0.59
1:A:115:ASN:OD1	1:A:118:ARG:NH2	2.35	0.58
1:A:290:ILE:HD13	1:A:334:ILE:HG23	1.85	0.58
1:B:179:ILE:HG13	1:B:225:ARG:NH1	2.19	0.58
1:D:70:LYS:NZ	1:D:70:LYS:HA	2.18	0.58
1:B:41:TYR:HB2	1:B:108:ARG:NH1	2.17	0.58
1:B:38:SER:HB3	2:B:501:TBR:BR1	2.59	0.57
1:B:15:ARG:HH12	1:B:81:ASP:HA	1.70	0.57
1:B:32:HIS:HB2	1:B:53:LEU:HD21	1.86	0.57
1:C:117:ILE:HG22	1:D:110:LEU:HD11	1.87	0.57
1:A:44:PRO:HB3	1:A:77:ILE:HG23	1.86	0.56
1:C:107:LYS:HZ3	1:D:124:SER:HA	1.69	0.56
1:A:179:ILE:HB	1:A:193:PHE:HB2	1.87	0.56
1:B:335:SER:HB2	1:B:381:ASP:HB2	1.88	0.56
1:C:119:GLU:OE2	1:C:119:GLU:N	2.39	0.56
1:B:108:ARG:HA	1:B:111:PHE:CD2	2.40	0.56
1:B:50:GLU:OE2	2:B:501:TBR:BR5	2.79	0.56
1:D:27:LYS:O	1:D:30:GLU:HG2	2.06	0.55
1:A:32:HIS:HB2	1:A:53:LEU:HD21	1.88	0.55
1:B:112:GLY:O	1:B:116:THR:OG1	2.20	0.55
1:A:301:LYS:HG2	1:A:345:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HD22	1:B:278:LYS:HB3	1.89	0.55
1:B:355:LEU:HA	1:B:372:ILE:HD13	1.89	0.54
1:D:73:LYS:HA	1:D:76:GLN:NE2	2.22	0.54
1:B:232:LEU:HD22	1:B:288:VAL:H	1.72	0.54
1:D:2:ASP:OD1	1:D:3:HIS:N	2.40	0.54
1:B:373:LYS:HB2	1:B:373:LYS:NZ	2.23	0.54
1:C:107:LYS:HZ3	1:D:124:SER:CA	2.19	0.54
1:A:73:LYS:HA	1:A:76:GLN:NE2	2.23	0.53
1:B:200:ILE:HD12	1:B:382:ALA:HB2	1.89	0.53
1:B:280:LEU:HD21	1:B:282:PHE:HE2	1.73	0.53
1:A:327:ARG:HH12	1:A:330:GLN:N	2.06	0.53
1:A:279:LYS:HD3	1:A:306:GLU:HG3	1.91	0.53
1:B:201:ILE:HG12	1:B:386:LEU:HB2	1.89	0.53
1:A:294:ARG:HA	1:A:341:LEU:HD22	1.91	0.53
1:B:64:GLU:OE1	1:B:68:ARG:NH2	2.38	0.53
1:D:73:LYS:HA	1:D:76:GLN:HE22	1.73	0.53
1:B:27:LYS:O	1:B:30:GLU:HG2	2.09	0.52
1:A:330:GLN:HB2	1:A:333:GLU:OE1	2.10	0.52
1:A:7:LEU:O	1:A:10:LEU:HG	2.10	0.52
1:D:7:LEU:O	1:D:10:LEU:HG	2.10	0.52
1:C:103:ASN:HA	1:C:106:ILE:HD12	1.91	0.52
1:B:99:GLU:O	1:B:103:ASN:ND2	2.40	0.51
1:D:41:TYR:HB2	1:D:108:ARG:NH1	2.25	0.51
1:A:280:LEU:HD21	1:A:282:PHE:HE2	1.75	0.51
1:A:4:LEU:HD22	1:D:4:LEU:HB3	1.92	0.51
1:A:13:ILE:HG22	1:A:101:ILE:HD11	1.93	0.51
1:A:82:LEU:HA	1:A:85:ILE:HD12	1.93	0.50
1:A:390:ARG:NH2	1:A:436:GLU:OE1	2.30	0.50
1:C:72:PRO:O	1:C:73:LYS:HG2	2.12	0.50
1:A:204:ARG:NH2	1:A:360:GLU:OE2	2.45	0.50
1:A:455:THR:OG1	1:A:465:GLU:O	2.30	0.50
1:B:18:LEU:O	1:B:22:VAL:HG23	2.11	0.50
1:D:61:PRO:HD2	1:D:66:PHE:CZ	2.47	0.50
1:A:7:LEU:HD23	1:A:10:LEU:HD21	1.93	0.49
1:A:201:ILE:O	1:A:353:VAL:N	2.42	0.49
1:B:205:PRO:HG3	1:B:354:GLN:CD	2.37	0.49
1:A:437:GLU:OE1	1:A:472:HIS:HE1	1.95	0.49
1:B:100:GLU:O	1:B:103:ASN:HB2	2.12	0.49
1:B:38:SER:HA	2:B:501:TBR:BRC	2.67	0.49
1:A:10:LEU:HA	1:A:13:ILE:HD12	1.95	0.49
1:A:250:ILE:HB	1:A:255:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:O	1:C:30:GLU:HG2	2.13	0.49
1:B:248:THR:HG21	1:B:268:LEU:HA	1.95	0.49
1:D:71:MET:SD	1:D:72:PRO:HD2	2.53	0.48
1:D:78:LYS:HB2	1:D:81:ASP:OD2	2.14	0.48
1:B:27:LYS:O	1:B:31:VAL:HG23	2.13	0.48
1:A:319:SER:HA	1:A:375:SER:N	2.28	0.48
1:A:294:ARG:HG3	1:A:341:LEU:HD13	1.96	0.48
1:A:419:TYR:O	1:A:423:ASN:ND2	2.41	0.48
1:B:387:PHE:HB2	1:B:441:ILE:HB	1.94	0.48
1:A:331:ILE:HG13	1:A:374:ASP:CG	2.39	0.48
1:A:153:ASN:HA	1:B:281:PHE:HA	1.95	0.48
1:B:195:LYS:HA	1:B:348:PRO:HD3	1.95	0.47
1:B:119:GLU:OE2	1:B:119:GLU:N	2.47	0.47
1:D:18:LEU:O	1:D:22:VAL:HG23	2.14	0.47
1:B:72:PRO:HB2	1:B:74:ASP:OD1	2.14	0.47
1:A:309:ILE:HD12	1:A:348:PRO:HG2	1.96	0.47
1:C:121:ALA:HB3	1:D:111:PHE:CE1	2.50	0.47
1:A:333:GLU:HA	1:A:336:ARG:NH1	2.30	0.47
1:C:7:LEU:O	1:C:10:LEU:HG	2.15	0.47
1:A:380:GLN:HG3	1:B:316:GLN:CG	2.45	0.47
1:B:94:ILE:HA	1:B:97:TYR:HD1	1.79	0.47
1:A:44:PRO:HA	1:A:47:LEU:HD12	1.97	0.46
1:C:71:MET:SD	1:C:72:PRO:HD2	2.54	0.46
1:C:72:PRO:C	1:C:74:ASP:H	2.24	0.46
1:A:11:GLN:O	1:A:15:ARG:HG3	2.15	0.46
1:A:153:ASN:N	1:B:282:PHE:H	2.13	0.46
1:B:25:ASN:O	1:B:28:ILE:HG22	2.16	0.46
1:A:366:ARG:HA	1:A:367:PRO:HD3	1.74	0.46
1:B:21:ILE:HD11	1:B:31:VAL:HG21	1.97	0.46
1:C:60:CYS:HA	1:C:61:PRO:HD3	1.82	0.46
1:A:18:LEU:HD22	1:A:48:PHE:CD1	2.51	0.46
1:B:47:LEU:CG	2:B:501:TBR:BR9	3.02	0.46
1:D:103:ASN:HA	1:D:106:ILE:HD12	1.96	0.46
1:B:294:ARG:HG3	1:B:341:LEU:HD13	1.97	0.46
1:D:27:LYS:O	1:D:31:VAL:HG23	2.16	0.45
1:A:79:GLU:OE2	1:A:82:LEU:HD23	2.16	0.45
1:B:199:VAL:O	1:B:350:ILE:HA	2.17	0.45
1:A:18:LEU:HD22	1:A:48:PHE:HD1	1.81	0.45
1:A:380:GLN:HG3	1:B:316:GLN:CD	2.41	0.45
1:A:468:PRO:O	1:A:472:HIS:HB2	2.17	0.45
1:B:111:PHE:CD1	1:B:111:PHE:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HA	1:A:7:LEU:HB2	1.99	0.45
1:A:64:GLU:HG2	1:A:86:PHE:CZ	2.52	0.45
1:D:0:THR:O	1:D:1:MET:HG2	2.17	0.45
1:A:15:ARG:NH1	1:A:84:ALA:HB3	2.32	0.44
1:A:103:ASN:O	1:A:107:LYS:HG3	2.17	0.44
1:C:32:HIS:HB2	1:C:53:LEU:HD21	1.99	0.44
1:A:27:LYS:O	1:A:30:GLU:HG2	2.17	0.44
1:D:72:PRO:O	1:D:73:LYS:HG2	2.17	0.44
1:A:316:GLN:OE1	1:A:354:GLN:HB3	2.18	0.44
1:A:36:GLU:H	1:A:39:ASP:CG	2.25	0.44
1:A:68:ARG:NH1	1:B:5:LYS:NZ	2.65	0.44
1:B:13:ILE:HG23	1:B:97:TYR:HD2	1.83	0.44
1:D:70:LYS:HA	1:D:70:LYS:HZ2	1.81	0.44
1:D:89:SER:HA	1:D:90:PRO:HD3	1.88	0.44
1:A:68:ARG:HH12	1:B:5:LYS:NZ	2.16	0.43
1:A:202:GLY:HA2	1:A:353:VAL:HB	2.00	0.43
1:A:320:GLY:N	1:A:375:SER:HB2	2.32	0.43
1:B:181:THR:HG21	1:B:186:LEU:HD23	2.00	0.43
1:B:379:GLU:OE2	1:B:381:ASP:N	2.50	0.43
1:C:104:ALA:O	1:C:108:ARG:HG3	2.17	0.43
1:A:155:LYS:HA	1:A:158:LEU:HD12	2.00	0.43
1:A:4:LEU:HA	1:A:7:LEU:HD12	1.98	0.43
1:A:100:GLU:O	1:A:103:ASN:HB2	2.19	0.43
1:A:467:MET:HA	1:A:468:PRO:HD3	1.79	0.43
1:A:18:LEU:O	1:A:22:VAL:HG23	2.19	0.43
1:D:97:TYR:HA	1:D:100:GLU:OE1	2.19	0.43
1:B:44:PRO:O	1:B:48:PHE:HB2	2.18	0.43
1:B:94:ILE:HA	1:B:97:TYR:CD1	2.54	0.43
1:B:390:ARG:HH21	1:B:436:GLU:CD	2.26	0.43
1:B:6:HIS:O	1:B:9:GLN:HB2	2.19	0.43
1:D:83:VAL:HA	1:D:86:PHE:HD2	1.83	0.43
1:A:359:LEU:HD11	1:A:367:PRO:HA	2.00	0.43
1:B:5:LYS:O	1:B:8:GLN:HG2	2.19	0.43
1:B:3:HIS:ND1	1:B:4:LEU:HD13	2.33	0.43
1:A:204:ARG:HB2	1:A:207:MET:HE3	2.00	0.43
1:A:248:THR:HG21	1:A:268:LEU:HA	2.02	0.42
1:C:71:MET:SD	1:C:76:GLN:HA	2.58	0.42
1:D:18:LEU:HD22	1:D:48:PHE:HD1	1.83	0.42
1:D:72:PRO:HB2	1:D:74:ASP:OD1	2.18	0.42
1:B:366:ARG:HA	1:B:367:PRO:HD3	1.83	0.42
1:B:152:ARG:HA	1:B:153:ASN:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:TYR:HD1	1:B:449:ALA:HB3	1.85	0.42
1:A:27:LYS:O	1:A:31:VAL:HG23	2.20	0.42
1:A:340:THR:O	1:A:344:GLU:HB2	2.18	0.42
1:A:422:VAL:HA	1:A:425:GLU:OE2	2.20	0.42
1:C:18:LEU:O	1:C:22:VAL:HG23	2.20	0.42
1:C:28:ILE:HG21	1:C:56:HIS:CG	2.54	0.42
1:A:4:LEU:O	1:A:8:GLN:HG3	2.19	0.42
1:B:60:CYS:HA	1:B:61:PRO:HD3	1.88	0.42
1:D:71:MET:SD	1:D:76:GLN:HA	2.59	0.42
1:B:7:LEU:HD23	1:B:10:LEU:HD13	2.00	0.42
1:B:204:ARG:HB2	1:B:207:MET:HE3	2.02	0.42
1:C:99:GLU:HG2	1:C:103:ASN:HD21	1.83	0.42
1:C:110:LEU:HD11	1:D:117:ILE:HG13	2.02	0.42
1:A:195:LYS:HB3	1:A:346:GLU:O	2.20	0.41
1:B:212:LEU:HD12	1:B:464:TYR:CD1	2.55	0.41
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.81	0.41
1:B:390:ARG:O	1:B:393:ILE:HG22	2.20	0.41
1:B:249:SER:HA	1:B:463:ARG:NH2	2.30	0.41
1:C:2:ASP:C	1:C:4:LEU:H	2.29	0.41
1:A:287:TYR:OH	1:A:326:GLU:O	2.38	0.41
1:C:64:GLU:HG2	1:C:86:PHE:CZ	2.54	0.41
1:A:42:TYR:CD2	1:A:44:PRO:HD2	2.55	0.41
1:A:60:CYS:HB3	1:A:66:PHE:CE1	2.56	0.41
1:A:385:VAL:HG23	1:A:444:LYS:HD3	2.03	0.41
1:B:313:ASP:HA	1:B:314:TYR:HA	1.75	0.41
1:C:14:GLU:OE1	1:C:45:ASN:ND2	2.53	0.41
1:A:386:LEU:HD23	1:A:442:VAL:HA	2.02	0.41
1:A:285:LYS:HA	1:A:285:LYS:HD2	1.82	0.41
1:A:293:ILE:O	1:A:297:LEU:HD13	2.20	0.41
1:D:48:PHE:HD2	1:D:77:ILE:HD13	1.85	0.41
1:A:199:VAL:HG13	1:A:384:ILE:HB	2.02	0.41
1:B:162:MET:SD	1:B:165:ILE:HD11	2.61	0.41
1:B:406:LEU:HD23	1:B:406:LEU:HA	1.93	0.41
1:A:378:ILE:O	1:A:380:GLN:HG2	2.20	0.40
1:B:40:PHE:CD1	1:B:46:GLY:HA2	2.56	0.40
1:B:42:TYR:HA	1:B:43:PRO:HD3	1.93	0.40
1:A:1:MET:O	1:A:5:LYS:HG3	2.20	0.40
1:C:80:GLU:HG3	1:C:81:ASP:H	1.86	0.40
1:A:179:ILE:HA	1:A:180:PRO:HD3	1.91	0.40
1:B:42:TYR:CD2	1:B:44:PRO:HD2	2.56	0.40
1:B:299:LYS:O	1:B:302:SER:OG	2.30	0.40

All (2) 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:A:121:ALA:O	1:B:107:LYS:NZ[9_555]	1.94	0.26
1:A:107:LYS:NZ	1:B:124:SER:O[9_555]	2.02	0.18

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	433/521 (83%)	423 (98%)	10 (2%)	0	100	100
1	B	422/521 (81%)	409 (97%)	13 (3%)	0	100	100
1	C	144/521 (28%)	138 (96%)	5 (4%)	1 (1%)	18	56
1	D	142/521 (27%)	136 (96%)	5 (4%)	1 (1%)	18	56
All	All	1141/2084 (55%)	1106 (97%)	33 (3%)	2 (0%)	43	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	SER
1	C	73	LYS

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	369/461 (80%)	360 (98%)	9 (2%)	43	64
1	B	356/461 (77%)	346 (97%)	10 (3%)	38	60
1	C	110/461 (24%)	108 (98%)	2 (2%)	51	68
1	D	110/461 (24%)	108 (98%)	2 (2%)	51	68
All	All	945/1844 (51%)	922 (98%)	23 (2%)	43	64

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	94	ILE
1	A	119	GLU
1	A	153	ASN
1	A	154	ILE
1	A	200	ILE
1	A	309	ILE
1	A	372	ILE
1	A	458	ASN
1	B	70	LYS
1	B	93	ASN
1	B	94	ILE
1	B	119	GLU
1	B	154	ILE
1	B	309	ILE
1	B	333	GLU
1	B	430	LYS
1	B	434	SER
1	B	458	ASN
1	C	70	LYS
1	C	119	GLU
1	D	70	LYS
1	D	94	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	32	HIS
1	A	93	ASN
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	194	ASN
1	A	292	GLN
1	A	380	GLN
1	A	429	HIS
1	B	188	ASN
1	B	194	ASN
1	B	264	GLN
1	B	292	GLN
1	B	380	GLN
1	C	32	HIS
1	C	103	ASN
1	D	8	GLN
1	D	115	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TBR	B	501	-	0,36,36	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	TBR	6	0

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	445/521 (85%)	0.51	48 (10%)	11 19	58, 291, 466, 550	0
1	B	434/521 (83%)	0.38	40 (9%)	14 22	75, 341, 550, 550	0
1	C	148/521 (28%)	0.36	14 (9%)	14 21	118, 270, 425, 539	0
1	D	146/521 (28%)	0.24	11 (7%)	20 26	114, 260, 386, 539	0
All	All	1173/2084 (56%)	0.41	113 (9%)	13 21	58, 301, 502, 550	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	SER	10.1
1	A	388	LEU	6.9
1	A	468	PRO	5.6
1	A	146	SER	5.3
1	B	228	ALA	5.0
1	A	22	VAL	5.0
1	A	469	ILE	5.0
1	A	91	ILE	4.9
1	B	240	ALA	4.7
1	B	93	ASN	4.5
1	A	358	SER	4.4
1	C	67	ILE	4.3
1	A	64	GLU	4.2
1	D	100	GLU	4.2
1	A	21	ILE	4.1
1	B	72	PRO	4.1
1	A	367	PRO	4.0
1	B	288	VAL	4.0
1	C	109	LYS	3.9
1	A	447	ASN	3.9
1	A	202	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	110	LEU	3.8
1	D	99	GLU	3.8
1	B	48	PHE	3.7
1	A	90	PRO	3.6
1	A	273	ASP	3.6
1	B	244	LEU	3.5
1	A	467	MET	3.5
1	D	235	VAL	3.5
1	A	89	SER	3.5
1	D	73	LYS	3.4
1	B	149	GLU	3.3
1	A	203	ALA	3.3
1	B	230	PHE	3.2
1	A	67	ILE	3.2
1	B	303	GLN	3.2
1	B	100	GLU	3.2
1	B	275	LEU	3.2
1	B	67	ILE	3.2
1	A	238	GLN	3.1
1	A	65	ASN	3.1
1	D	247	THR	3.1
1	B	247	LEU	3.1
1	B	268	LEU	3.0
1	B	152	ARG	3.0
1	A	132	LEU	2.9
1	B	0	THR	2.9
1	C	113	LEU	2.9
1	C	141	ALA	2.9
1	D	239	VAL	2.9
1	C	116	THR	2.8
1	B	218	LEU	2.8
1	A	470	ASP	2.8
1	B	292	GLN	2.8
1	A	387	PHE	2.8
1	A	195	LYS	2.8
1	C	120	GLN	2.8
1	D	41	TYR	2.8
1	B	270	LYS	2.7
1	D	98	VAL	2.7
1	A	349	ILE	2.7
1	B	267	ASN	2.7
1	C	135	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	65	ASN	2.6
1	A	425	GLU	2.6
1	A	386	LEU	2.6
1	B	318	MET	2.6
1	A	62	ILE	2.6
1	B	239	LEU	2.6
1	A	311	PHE	2.5
1	B	259	ARG	2.5
1	C	12	ASN	2.5
1	C	138	GLU	2.5
1	B	300	LEU	2.5
1	A	216	MET	2.5
1	C	5	LYS	2.5
1	A	200	ILE	2.4
1	B	75	LYS	2.4
1	B	271	CYS	2.4
1	A	322	LYS	2.4
1	D	0	THR	2.4
1	A	20	GLY	2.3
1	A	353	VAL	2.3
1	A	239	LEU	2.3
1	B	206	SER	2.3
1	A	472	HIS	2.3
1	A	78	LYS	2.3
1	B	376	GLY	2.3
1	A	473	LEU	2.3
1	B	256	GLU	2.3
1	A	393	ILE	2.3
1	D	79	GLU	2.2
1	B	311	PHE	2.2
1	A	48	PHE	2.2
1	C	0	THR	2.2
1	B	462	THR	2.2
1	B	146	SER	2.2
1	B	317	LEU	2.2
1	B	74	ASP	2.2
1	A	201	ILE	2.2
1	B	229	VAL	2.1
1	A	27	LYS	2.1
1	A	131	ILE	2.1
1	A	421	LYS	2.1
1	C	68	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	310	ALA	2.1
1	B	372	ILE	2.1
1	B	148	ILE	2.1
1	A	369	LEU	2.1
1	A	315	LEU	2.0
1	D	34	VAL	2.0
1	A	390	ARG	2.0
1	B	346	GLU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TBR	B	501	18/18	0.69	0.09	550,550,550,550	18

6.5 Other polymers [i](#)

There are no such residues in this entry.