



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:52 AM UTC

PDB ID : 7QXM / pdb_00007qxm
Title : Crystal structure of the Vibrio cholerae replicative helicase (DnaB)
Authors : Legrand, P.; Quevillon-Cheruel, S.; Walbott, H.; Cargemel, C.
Deposited on : 2022-01-26
Resolution : 3.80 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

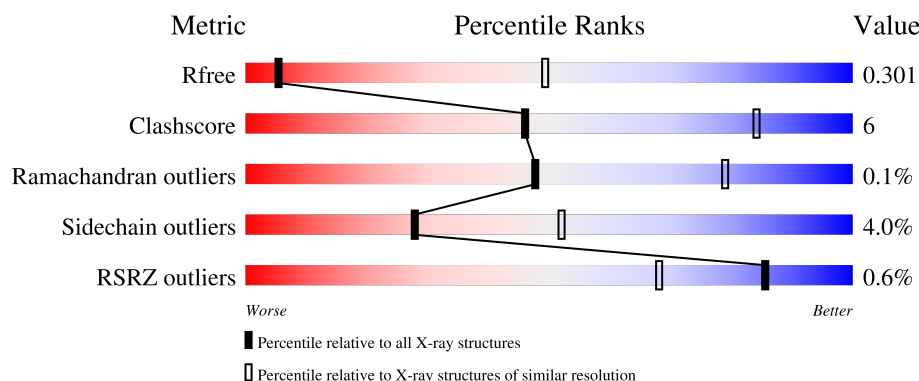
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	474	
1	B	474	
1	C	474	
1	D	474	
1	E	474	

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Mol	Chain	Length	Quality of chain
1	F	474	78% 14% • 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20679 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	440	Total	C	N	O	S	0	0	0
			3433	2139	603	676	15			
1	B	440	Total	C	N	O	S	0	0	0
			3436	2142	603	676	15			
1	C	448	Total	C	N	O	S	0	0	0
			3493	2177	612	689	15			
1	D	439	Total	C	N	O	S	0	0	0
			3428	2136	602	675	15			
1	E	444	Total	C	N	O	S	0	0	0
			3460	2158	607	680	15			
1	F	440	Total	C	N	O	S	0	0	0
			3429	2136	603	675	15			

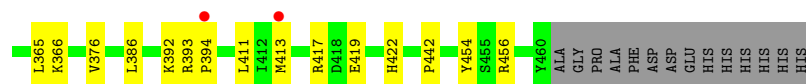
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP A0A085R2T8
A	470	HIS	-	expression tag	UNP A0A085R2T8
A	471	HIS	-	expression tag	UNP A0A085R2T8
A	472	HIS	-	expression tag	UNP A0A085R2T8
A	473	HIS	-	expression tag	UNP A0A085R2T8
A	474	HIS	-	expression tag	UNP A0A085R2T8
B	469	HIS	-	expression tag	UNP A0A085R2T8
B	470	HIS	-	expression tag	UNP A0A085R2T8
B	471	HIS	-	expression tag	UNP A0A085R2T8
B	472	HIS	-	expression tag	UNP A0A085R2T8
B	473	HIS	-	expression tag	UNP A0A085R2T8
B	474	HIS	-	expression tag	UNP A0A085R2T8
C	469	HIS	-	expression tag	UNP A0A085R2T8
C	470	HIS	-	expression tag	UNP A0A085R2T8
C	471	HIS	-	expression tag	UNP A0A085R2T8
C	472	HIS	-	expression tag	UNP A0A085R2T8
C	473	HIS	-	expression tag	UNP A0A085R2T8

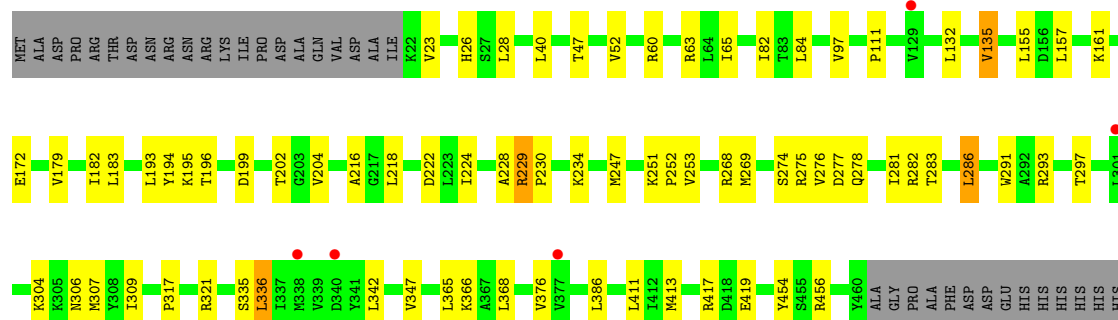
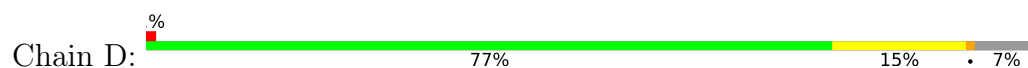
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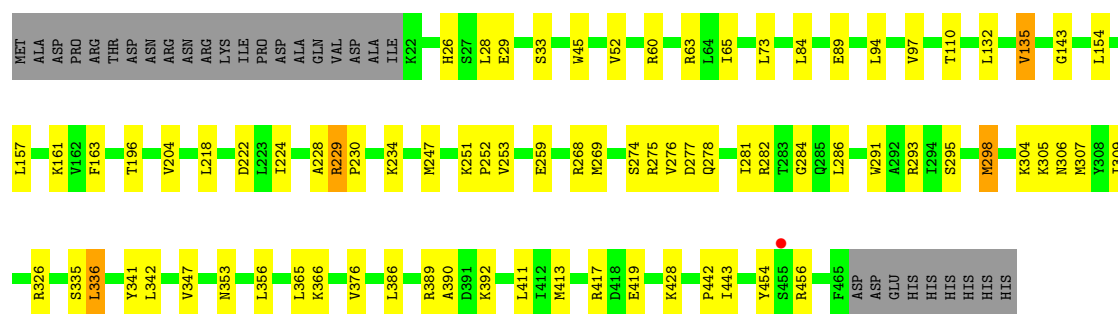
Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	expression tag	UNP A0A085R2T8
D	469	HIS	-	expression tag	UNP A0A085R2T8
D	470	HIS	-	expression tag	UNP A0A085R2T8
D	471	HIS	-	expression tag	UNP A0A085R2T8
D	472	HIS	-	expression tag	UNP A0A085R2T8
D	473	HIS	-	expression tag	UNP A0A085R2T8
D	474	HIS	-	expression tag	UNP A0A085R2T8
E	469	HIS	-	expression tag	UNP A0A085R2T8
E	470	HIS	-	expression tag	UNP A0A085R2T8
E	471	HIS	-	expression tag	UNP A0A085R2T8
E	472	HIS	-	expression tag	UNP A0A085R2T8
E	473	HIS	-	expression tag	UNP A0A085R2T8
E	474	HIS	-	expression tag	UNP A0A085R2T8
F	469	HIS	-	expression tag	UNP A0A085R2T8
F	470	HIS	-	expression tag	UNP A0A085R2T8
F	471	HIS	-	expression tag	UNP A0A085R2T8
F	472	HIS	-	expression tag	UNP A0A085R2T8
F	473	HIS	-	expression tag	UNP A0A085R2T8
F	474	HIS	-	expression tag	UNP A0A085R2T8



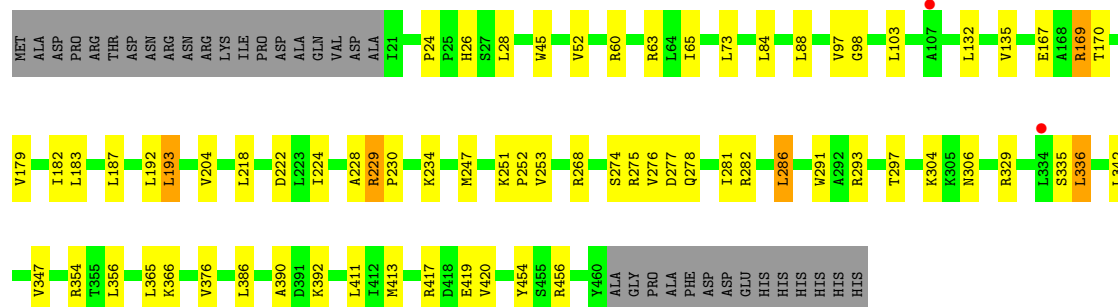
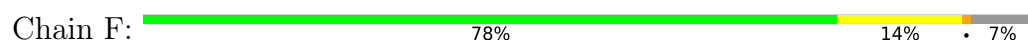
• Molecule 1: Replicative DNA helicase



• Molecule 1: Replicative DNA helicase



• Molecule 1: Replicative DNA helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.23Å 150.10Å 188.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.63 – 3.80 32.63 – 3.80	Depositor EDS
% Data completeness (in resolution range)	72.7 (32.63-3.80) 72.5 (32.63-3.80)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.75Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.266 , 0.274 0.294 , 0.301	Depositor DCC
R_{free} test set	1408 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	152.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 125.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20679	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.48	0/3482	0.88	0/4708
1	B	0.48	0/3485	0.89	0/4712
1	C	0.49	0/3543	0.89	0/4793
1	D	0.49	0/3477	0.88	0/4701
1	E	0.48	0/3511	0.88	0/4748
1	F	0.49	0/3477	0.89	1/4701 (0.0%)
All	All	0.49	0/20975	0.89	1/28363 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	24	PRO	N-CA-C	5.31	115.57	110.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3433	0	3441	46	0
1	B	3436	0	3447	41	0
1	C	3493	0	3500	43	0
1	D	3428	0	3436	52	0
1	E	3460	0	3465	52	0
1	F	3429	0	3440	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20679	0	20729	240	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 6.

All (240) 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:F:60:ARG:HH11	1:F:63:ARG:HH12	1.10	0.99
1:D:60:ARG:HH11	1:D:63:ARG:HH12	1.11	0.99
1:A:60:ARG:HH11	1:A:63:ARG:HH12	1.12	0.96
1:E:60:ARG:HH11	1:E:63:ARG:HH12	1.11	0.94
1:C:60:ARG:HH11	1:C:63:ARG:HH12	1.10	0.93
1:F:60:ARG:HH11	1:F:63:ARG:NH1	1.73	0.87
1:A:60:ARG:HH11	1:A:63:ARG:NH1	1.73	0.87
1:D:60:ARG:HH11	1:D:63:ARG:NH1	1.73	0.86
1:E:60:ARG:HH11	1:E:63:ARG:NH1	1.74	0.86
1:C:60:ARG:HH11	1:C:63:ARG:NH1	1.74	0.85
1:C:60:ARG:NH1	1:C:63:ARG:HH12	1.77	0.83
1:E:60:ARG:NH1	1:E:63:ARG:HH12	1.78	0.82
1:F:60:ARG:NH1	1:F:63:ARG:HH12	1.76	0.81
1:D:60:ARG:NH1	1:D:63:ARG:HH12	1.78	0.81
1:A:60:ARG:NH1	1:A:63:ARG:HH12	1.79	0.80
1:A:390:ALA:HA	1:A:392:LYS:NZ	2.02	0.74
1:D:196:THR:HB	1:D:199:ASP:HB2	1.70	0.74
1:D:47:THR:HG22	1:E:326:ARG:HE	1.52	0.72
1:D:222:ASP:HA	1:D:366:LYS:NZ	2.06	0.70
1:B:222:ASP:HA	1:B:366:LYS:NZ	2.06	0.70
1:D:222:ASP:HA	1:D:366:LYS:HZ2	1.55	0.70
1:F:222:ASP:HA	1:F:366:LYS:NZ	2.06	0.69
1:A:222:ASP:HA	1:A:366:LYS:NZ	2.07	0.69
1:C:222:ASP:HA	1:C:366:LYS:NZ	2.07	0.69
1:E:222:ASP:HA	1:E:366:LYS:NZ	2.07	0.69
1:A:222:ASP:HA	1:A:366:LYS:HZ2	1.58	0.68
1:D:183:LEU:HD21	1:E:298:MET:HG3	1.75	0.68
1:D:286:LEU:HD11	1:D:291:TRP:CD1	2.29	0.68
1:A:390:ALA:HA	1:A:392:LYS:HZ3	1.59	0.67
1:D:82:ILE:HD11	1:E:29:GLU:HB2	1.79	0.65
1:E:26:HIS:CD2	1:E:28:LEU:HG	2.32	0.64
1:D:268:ARG:HH21	1:D:282:ARG:HH22	1.46	0.64
1:B:268:ARG:HH21	1:B:282:ARG:HH22	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:HIS:CD2	1:D:28:LEU:HG	2.32	0.64
1:B:26:HIS:CD2	1:B:28:LEU:HG	2.33	0.64
1:C:60:ARG:NH1	1:C:63:ARG:NH1	2.43	0.63
1:A:204:VAL:HB	1:A:218:LEU:HB2	1.81	0.63
1:A:268:ARG:HH21	1:A:282:ARG:HH22	1.47	0.63
1:B:204:VAL:HB	1:B:218:LEU:HB2	1.81	0.63
1:F:228:ALA:HB3	1:F:234:LYS:HB3	1.81	0.63
1:E:268:ARG:HH21	1:E:282:ARG:HH22	1.46	0.63
1:E:274:SER:HB3	1:E:293:ARG:HB3	1.81	0.62
1:D:204:VAL:HB	1:D:218:LEU:HB2	1.81	0.62
1:E:204:VAL:HB	1:E:218:LEU:HB2	1.81	0.62
1:B:82:ILE:HD11	1:C:29:GLU:HB2	1.80	0.62
1:A:26:HIS:CD2	1:A:28:LEU:HG	2.35	0.62
1:C:268:ARG:HH21	1:C:282:ARG:HH22	1.48	0.62
1:F:204:VAL:HB	1:F:218:LEU:HB2	1.81	0.62
1:C:204:VAL:HB	1:C:218:LEU:HB2	1.81	0.61
1:A:167:GLU:HG3	1:B:326:ARG:HD3	1.81	0.61
1:D:47:THR:CG2	1:E:326:ARG:HE	2.14	0.61
1:F:222:ASP:HA	1:F:366:LYS:HZ2	1.66	0.60
1:A:286:LEU:HD11	1:A:291:TRP:CD1	2.36	0.59
1:F:365:LEU:HD12	1:F:376:VAL:HG11	1.85	0.59
1:E:229:ARG:HG3	1:E:230:PRO:HD2	1.84	0.59
1:C:442:PRO:HB3	1:D:283:THR:HA	1.84	0.59
1:B:365:LEU:HD12	1:B:376:VAL:HG11	1.85	0.59
1:D:60:ARG:NH1	1:D:63:ARG:NH1	2.43	0.59
1:F:286:LEU:HD11	1:F:291:TRP:CD1	2.37	0.59
1:A:365:LEU:HD12	1:A:376:VAL:HG11	1.85	0.59
1:D:26:HIS:HD2	1:D:28:LEU:HG	1.67	0.58
1:D:229:ARG:HG3	1:D:230:PRO:HD2	1.86	0.58
1:D:365:LEU:HD12	1:D:376:VAL:HG11	1.85	0.58
1:F:60:ARG:NH1	1:F:63:ARG:NH1	2.42	0.58
1:E:365:LEU:HD12	1:E:376:VAL:HG11	1.84	0.58
1:D:194:TYR:OH	1:E:291:TRP:NE1	2.36	0.58
1:F:229:ARG:HG3	1:F:230:PRO:HD2	1.86	0.58
1:A:26:HIS:HD2	1:A:28:LEU:HG	1.68	0.58
1:C:365:LEU:HD12	1:C:376:VAL:HG11	1.85	0.58
1:E:222:ASP:HA	1:E:366:LYS:HZ3	1.66	0.58
1:E:60:ARG:NH1	1:E:63:ARG:NH1	2.45	0.58
1:B:72:ILE:HD13	1:B:83:THR:HG22	1.87	0.57
1:B:26:HIS:HD2	1:B:28:LEU:HG	1.69	0.57
1:C:222:ASP:HA	1:C:366:LYS:HZ2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:NH1	1:A:63:ARG:NH1	2.44	0.56
1:B:228:ALA:HB3	1:B:234:LYS:HB3	1.87	0.56
1:D:277:ASP:HA	1:D:454:TYR:HB3	1.88	0.56
1:E:277:ASP:HA	1:E:454:TYR:HB3	1.87	0.56
1:B:277:ASP:HA	1:B:454:TYR:HB3	1.88	0.56
1:F:277:ASP:HA	1:F:454:TYR:HB3	1.87	0.56
1:C:166:ALA:HB2	1:D:155:LEU:HD21	1.87	0.56
1:C:277:ASP:HA	1:C:454:TYR:HB3	1.87	0.56
1:E:228:ALA:HB3	1:E:234:LYS:HB3	1.87	0.56
1:E:26:HIS:HD2	1:E:28:LEU:HG	1.69	0.56
1:B:222:ASP:HA	1:B:366:LYS:HZ2	1.71	0.56
1:A:277:ASP:HA	1:A:454:TYR:HB3	1.88	0.55
1:C:228:ALA:HB3	1:C:234:LYS:HB3	1.89	0.55
1:A:228:ALA:HB3	1:A:234:LYS:HB3	1.88	0.55
1:C:276:VAL:HG23	1:C:281:ILE:HD11	1.88	0.55
1:C:442:PRO:CB	1:D:283:THR:HA	2.37	0.54
1:D:276:VAL:HG23	1:D:281:ILE:HD11	1.89	0.54
1:C:33:SER:HA	1:C:110:THR:HG22	1.89	0.54
1:A:270:LEU:HD21	1:A:298:MET:HE1	1.89	0.54
1:D:321:ARG:HG2	1:D:368:LEU:HD13	1.90	0.54
1:E:163:PHE:CZ	1:F:329:ARG:NH2	2.76	0.54
1:D:228:ALA:HB3	1:D:234:LYS:HB3	1.89	0.53
1:E:276:VAL:HG23	1:E:281:ILE:HD11	1.90	0.53
1:B:286:LEU:HD11	1:B:291:TRP:CD1	2.43	0.53
1:D:47:THR:HG22	1:E:326:ARG:NE	2.22	0.53
1:F:276:VAL:HG23	1:F:281:ILE:HD11	1.89	0.53
1:B:274:SER:HB3	1:B:293:ARG:HB3	1.89	0.53
1:A:276:VAL:HG23	1:A:281:ILE:HD11	1.89	0.53
1:D:274:SER:HB3	1:D:293:ARG:HB3	1.91	0.53
1:C:135:VAL:HG13	1:C:161:LYS:HB3	1.91	0.52
1:B:229:ARG:HG3	1:B:230:PRO:HD2	1.92	0.52
1:E:196:THR:HG21	1:E:442:PRO:HD3	1.90	0.52
1:A:253:VAL:HG12	1:A:336:LEU:HB3	1.92	0.52
1:C:44:ARG:HG3	1:C:116:ILE:HD13	1.90	0.52
1:D:194:TYR:CZ	1:E:291:TRP:NE1	2.77	0.51
1:D:252:PRO:HA	1:D:306:ASN:HB3	1.92	0.51
1:A:229:ARG:HG3	1:A:230:PRO:HD2	1.91	0.51
1:F:169:ARG:HD3	1:F:170:THR:HG23	1.90	0.51
1:D:253:VAL:HG12	1:D:336:LEU:HB3	1.93	0.51
1:E:143:GLY:HA2	1:E:154:LEU:HD21	1.91	0.51
1:E:252:PRO:HA	1:E:306:ASN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:VAL:HG12	1:E:336:LEU:HB3	1.92	0.51
1:F:253:VAL:HG12	1:F:336:LEU:HB3	1.92	0.51
1:A:128:LEU:HB2	1:B:151:ALA:HB1	1.91	0.51
1:C:229:ARG:HG3	1:C:230:PRO:HD2	1.92	0.50
1:C:253:VAL:HG12	1:C:336:LEU:HB3	1.94	0.50
1:B:196:THR:HB	1:B:199:ASP:HB2	1.93	0.50
1:D:194:TYR:HH	1:E:291:TRP:NE1	2.09	0.50
1:A:390:ALA:HA	1:A:392:LYS:HZ2	1.75	0.50
1:B:253:VAL:HG12	1:B:336:LEU:HB3	1.92	0.50
1:F:390:ALA:HA	1:F:392:LYS:HE2	1.94	0.49
1:A:305:LYS:HA	1:F:179:VAL:HG21	1.93	0.49
1:B:222:ASP:HA	1:B:366:LYS:HZ1	1.75	0.49
1:E:353:ASN:HD21	1:F:354:ARG:HB2	1.77	0.49
1:F:252:PRO:HA	1:F:306:ASN:HB3	1.94	0.49
1:A:196:THR:HG21	1:A:442:PRO:HD3	1.93	0.49
1:C:274:SER:HB3	1:C:293:ARG:HB3	1.95	0.49
1:B:252:PRO:HA	1:B:306:ASN:HB3	1.94	0.48
1:E:295:SER:HA	1:E:298:MET:HE2	1.93	0.48
1:F:274:SER:HB3	1:F:293:ARG:HB3	1.94	0.48
1:A:284:GLY:HA3	1:F:193:LEU:HB3	1.96	0.48
1:B:81:LEU:HD22	1:B:104:ALA:HA	1.95	0.48
1:C:247:MET:HA	1:C:304:LYS:HD3	1.95	0.48
1:C:392:LYS:NZ	1:C:422:HIS:NE2	2.55	0.48
1:B:65:ILE:HG23	1:B:84:LEU:HD21	1.95	0.48
1:E:247:MET:HA	1:E:304:LYS:HD3	1.95	0.48
1:A:286:LEU:CD1	1:A:291:TRP:CD1	2.96	0.48
1:B:247:MET:HA	1:B:304:LYS:HD3	1.97	0.47
1:B:45:TRP:HB2	1:B:73:LEU:HD13	1.96	0.47
1:B:190:ILE:HA	1:B:193:LEU:HD12	1.97	0.47
1:D:269:MET:HE1	1:D:307:MET:HG3	1.97	0.47
1:E:135:VAL:HG13	1:E:161:LYS:HB3	1.95	0.47
1:B:135:VAL:HG13	1:B:161:LYS:HB3	1.96	0.47
1:D:247:MET:HA	1:D:304:LYS:HD3	1.97	0.47
1:F:286:LEU:CD1	1:F:291:TRP:CD1	2.98	0.47
1:A:80:ASP:H	1:A:83:THR:HB	1.79	0.47
1:B:194:TYR:CZ	1:C:291:TRP:NE1	2.80	0.47
1:B:286:LEU:CD1	1:B:291:TRP:CD1	2.98	0.47
1:E:163:PHE:HZ	1:F:329:ARG:NH2	2.11	0.47
1:E:269:MET:HE1	1:E:307:MET:HG3	1.97	0.47
1:F:224:ILE:HG12	1:F:411:LEU:HD23	1.97	0.47
1:A:224:ILE:HG12	1:A:411:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:VAL:HG13	1:D:161:LYS:HB3	1.95	0.47
1:F:247:MET:HA	1:F:304:LYS:HD3	1.97	0.47
1:D:252:PRO:HB3	1:D:306:ASN:HA	1.97	0.47
1:C:222:ASP:HA	1:C:366:LYS:HZ1	1.78	0.47
1:A:269:MET:HE1	1:A:307:MET:HG3	1.97	0.46
1:A:309:ILE:HD12	1:F:182:ILE:HD13	1.97	0.46
1:D:286:LEU:CD1	1:D:291:TRP:CD1	2.96	0.46
1:E:224:ILE:HG12	1:E:411:LEU:HD23	1.97	0.46
1:C:224:ILE:HG12	1:C:411:LEU:HD23	1.97	0.46
1:D:317:PRO:HG2	1:D:347:VAL:HB	1.96	0.46
1:D:224:ILE:HG12	1:D:411:LEU:HD23	1.97	0.46
1:B:417:ARG:HG2	1:B:419:GLU:HG2	1.98	0.46
1:D:417:ARG:HG2	1:D:419:GLU:HG2	1.98	0.46
1:B:269:MET:HE1	1:B:307:MET:HG3	1.97	0.46
1:C:417:ARG:HG2	1:C:419:GLU:HG2	1.98	0.46
1:A:155:LEU:HD21	1:B:166:ALA:HB2	1.97	0.46
1:A:179:VAL:HG21	1:B:305:LYS:HA	1.98	0.45
1:B:224:ILE:HG12	1:B:411:LEU:HD23	1.97	0.45
1:D:65:ILE:HG23	1:D:84:LEU:HD21	1.98	0.45
1:E:259:GLU:HB2	1:E:341:TYR:HD2	1.81	0.45
1:E:417:ARG:HG2	1:E:419:GLU:HG2	1.98	0.45
1:F:222:ASP:HA	1:F:366:LYS:HZ1	1.80	0.45
1:A:81:LEU:HD22	1:A:104:ALA:HA	1.99	0.45
1:A:275:ARG:HH21	1:A:456:ARG:NH1	2.15	0.45
1:B:276:VAL:HG23	1:B:281:ILE:HD11	1.97	0.45
1:A:417:ARG:HG2	1:A:419:GLU:HG2	1.98	0.45
1:F:275:ARG:HH21	1:F:456:ARG:NH1	2.15	0.45
1:A:298:MET:HE3	1:F:187:LEU:HD21	1.98	0.45
1:C:259:GLU:HB2	1:C:341:TYR:HD2	1.82	0.45
1:B:275:ARG:HH21	1:B:456:ARG:NH1	2.15	0.45
1:A:72:ILE:HD13	1:A:83:THR:HG22	1.99	0.45
1:A:132:LEU:HD11	1:B:155:LEU:HA	1.98	0.45
1:E:222:ASP:HA	1:E:366:LYS:HZ2	1.80	0.45
1:F:417:ARG:HG2	1:F:419:GLU:HG2	1.98	0.45
1:A:135:VAL:HG13	1:A:161:LYS:HB3	1.98	0.44
1:A:411:LEU:HD21	1:A:413:MET:HE3	2.00	0.44
1:E:275:ARG:HH21	1:E:456:ARG:NH1	2.15	0.44
1:C:411:LEU:HD21	1:C:413:MET:HE3	1.99	0.44
1:D:179:VAL:HG21	1:E:305:LYS:HA	1.98	0.44
1:A:301:LEU:HD23	1:F:183:LEU:HD11	1.98	0.44
1:D:411:LEU:HD21	1:D:413:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HB3	1:E:284:GLY:HA3	1.98	0.44
1:E:390:ALA:HA	1:E:392:LYS:HE2	1.99	0.44
1:D:275:ARG:HH21	1:D:456:ARG:NH1	2.15	0.44
1:E:65:ILE:HG23	1:E:84:LEU:HD21	2.00	0.44
1:C:275:ARG:HH21	1:C:456:ARG:NH1	2.15	0.44
1:C:182:ILE:HG21	1:D:309:ILE:HD12	1.99	0.43
1:F:268:ARG:HH21	1:F:282:ARG:HH22	1.66	0.43
1:F:411:LEU:HD21	1:F:413:MET:HE3	2.00	0.43
1:B:411:LEU:HD21	1:B:413:MET:HE3	2.00	0.43
1:C:135:VAL:HG22	1:C:161:LYS:HD2	2.00	0.43
1:E:411:LEU:HD21	1:E:413:MET:HE3	2.00	0.43
1:C:251:LYS:HB2	1:C:335:SER:HB3	2.01	0.43
1:D:202:THR:OG1	1:D:216:ALA:O	2.37	0.43
1:D:182:ILE:HD13	1:E:309:ILE:HD12	2.00	0.43
1:D:251:LYS:HB2	1:D:335:SER:HB3	2.01	0.43
1:F:26:HIS:CD2	1:F:28:LEU:HG	2.54	0.43
1:F:251:LYS:HB2	1:F:335:SER:HB3	2.00	0.43
1:C:26:HIS:HD2	1:C:28:LEU:HG	1.83	0.42
1:A:353:ASN:HD21	1:B:354:ARG:HB2	1.84	0.42
1:B:182:ILE:HD13	1:C:309:ILE:HD12	2.00	0.42
1:A:251:LYS:HB2	1:A:335:SER:HB3	2.00	0.42
1:E:251:LYS:HB2	1:E:335:SER:HB3	2.01	0.42
1:E:389:ARG:O	1:F:420:VAL:O	2.37	0.42
1:B:194:TYR:CE2	1:C:291:TRP:NE1	2.82	0.42
1:F:88:LEU:HD12	1:F:103:LEU:HD11	2.01	0.42
1:B:251:LYS:HB2	1:B:335:SER:HB3	2.01	0.42
1:E:89:GLU:HB2	1:E:94:LEU:HD22	2.00	0.42
1:F:45:TRP:HB2	1:F:73:LEU:HD13	2.02	0.42
1:F:65:ILE:HG23	1:F:84:LEU:HD21	2.01	0.41
1:C:103:LEU:HA	1:C:106:LEU:HD12	2.02	0.41
1:C:252:PRO:HA	1:C:306:ASN:HB3	2.02	0.41
1:C:45:TRP:HB2	1:C:73:LEU:HD13	2.03	0.41
1:C:65:ILE:HD11	1:C:97:VAL:HG13	2.02	0.41
1:C:392:LYS:HZ3	1:C:422:HIS:CE1	2.37	0.40
1:C:393:ARG:HA	1:C:394:PRO:HD3	1.97	0.40
1:E:45:TRP:HB2	1:E:73:LEU:HD13	2.03	0.40
1:E:443:ILE:HD11	1:F:282:ARG:HD3	2.02	0.40
1:A:82:ILE:HD12	1:A:82:ILE:HA	1.96	0.40
1:D:286:LEU:HD11	1:D:291:TRP:CG	2.56	0.40
1:E:33:SER:HB3	1:E:110:THR:HG21	2.02	0.40
1:A:65:ILE:HG23	1:A:84:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:CD1	1:D:111:PRO:HA	2.52	0.40
1:D:196:THR:CB	1:D:199:ASP:HB2	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/474 (92%)	418 (95%)	20 (5%)	0	100	100
1	B	438/474 (92%)	413 (94%)	25 (6%)	0	100	100
1	C	446/474 (94%)	420 (94%)	25 (6%)	1 (0%)	43	73
1	D	437/474 (92%)	409 (94%)	27 (6%)	1 (0%)	43	73
1	E	442/474 (93%)	417 (94%)	25 (6%)	0	100	100
1	F	438/474 (92%)	410 (94%)	27 (6%)	1 (0%)	43	73
All	All	2639/2844 (93%)	2487 (94%)	149 (6%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	172	GLU
1	C	98	GLY
1	F	98	GLY

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	374/403 (93%)	362 (97%)	12 (3%)	34	56
1	B	375/403 (93%)	359 (96%)	16 (4%)	26	50
1	C	381/403 (94%)	365 (96%)	16 (4%)	26	50
1	D	374/403 (93%)	360 (96%)	14 (4%)	30	54
1	E	376/403 (93%)	361 (96%)	15 (4%)	28	52
1	F	374/403 (93%)	357 (96%)	17 (4%)	24	48
All	All	2254/2418 (93%)	2164 (96%)	90 (4%)	28	52

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	135	VAL
1	A	157	LEU
1	A	278	GLN
1	A	286	LEU
1	A	297	THR
1	A	336	LEU
1	A	342	LEU
1	A	347	VAL
1	A	356	LEU
1	A	386	LEU
1	A	428	LYS
1	B	23	VAL
1	B	52	VAL
1	B	82	ILE
1	B	132	LEU
1	B	135	VAL
1	B	157	LEU
1	B	179	VAL
1	B	183	LEU
1	B	278	GLN
1	B	285	GLN
1	B	297	THR
1	B	336	LEU
1	B	342	LEU
1	B	347	VAL
1	B	356	LEU
1	B	395	VAL

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Mol	Chain	Res	Type
1	C	52	VAL
1	C	97	VAL
1	C	105	ASP
1	C	132	LEU
1	C	135	VAL
1	C	150	ASN
1	C	174	GLU
1	C	278	GLN
1	C	286	LEU
1	C	291	TRP
1	C	297	THR
1	C	336	LEU
1	C	342	LEU
1	C	347	VAL
1	C	356	LEU
1	C	386	LEU
1	D	23	VAL
1	D	52	VAL
1	D	97	VAL
1	D	132	LEU
1	D	135	VAL
1	D	157	LEU
1	D	195	LYS
1	D	229	ARG
1	D	278	GLN
1	D	286	LEU
1	D	297	THR
1	D	336	LEU
1	D	342	LEU
1	D	386	LEU
1	E	52	VAL
1	E	97	VAL
1	E	132	LEU
1	E	135	VAL
1	E	157	LEU
1	E	229	ARG
1	E	278	GLN
1	E	286	LEU
1	E	298	MET
1	E	336	LEU
1	E	342	LEU
1	E	347	VAL

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Mol	Chain	Res	Type
1	E	356	LEU
1	E	386	LEU
1	E	428	LYS
1	F	52	VAL
1	F	97	VAL
1	F	132	LEU
1	F	135	VAL
1	F	167	GLU
1	F	169	ARG
1	F	192	LEU
1	F	193	LEU
1	F	229	ARG
1	F	278	GLN
1	F	286	LEU
1	F	297	THR
1	F	336	LEU
1	F	342	LEU
1	F	347	VAL
1	F	356	LEU
1	F	386	LEU

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	306	ASN
1	A	343	GLN
1	A	422	HIS
1	A	438	GLN
1	B	42	ASN
1	B	306	ASN
1	B	343	GLN
1	B	422	HIS
1	B	438	GLN
1	C	17	GLN
1	C	306	ASN
1	C	343	GLN
1	C	438	GLN
1	D	306	ASN
1	D	331	HIS
1	D	422	HIS
1	D	438	GLN
1	E	115	ASN

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Mol	Chain	Res	Type
1	E	306	ASN
1	E	422	HIS
1	E	438	GLN
1	F	306	ASN
1	F	343	GLN
1	F	438	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

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	440/474 (92%)	-0.15	3 (0%) 84 65	123, 171, 189, 194	0
1	B	440/474 (92%)	-0.17	0 100 100	116, 186, 228, 232	0
1	C	448/474 (94%)	0.03	5 (1%) 78 56	121, 194, 221, 230	0
1	D	439/474 (92%)	0.04	5 (1%) 78 56	120, 204, 246, 253	0
1	E	444/474 (93%)	-0.12	1 (0%) 91 81	141, 168, 208, 219	0
1	F	440/474 (92%)	-0.08	2 (0%) 87 71	125, 183, 205, 214	0
All	All	2651/2844 (93%)	-0.07	16 (0%) 85 68	116, 179, 228, 253	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	LEU	3.6
1	C	226	VAL	3.4
1	D	129	VAL	3.0
1	D	340	ASP	2.8
1	A	431	ALA	2.6
1	C	413	MET	2.6
1	D	338	MET	2.6
1	F	334	LEU	2.5
1	C	243	GLU	2.3
1	D	301	LEU	2.2
1	E	455	SER	2.2
1	C	394	PRO	2.2
1	A	307	MET	2.1
1	A	112	SER	2.1
1	F	107	ALA	2.1
1	D	377	VAL	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.