



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:09 AM UTC

PDB ID : 4A1F / pdb_00004a1f
Title : Crystal structure of C-terminal domain of Helicobacter pylori DnaB Helicase
Authors : Stelter, M.; Kapp, U.; Timmins, J.; Terradot, L.
Deposited on : 2011-09-14
Resolution : 2.50 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
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

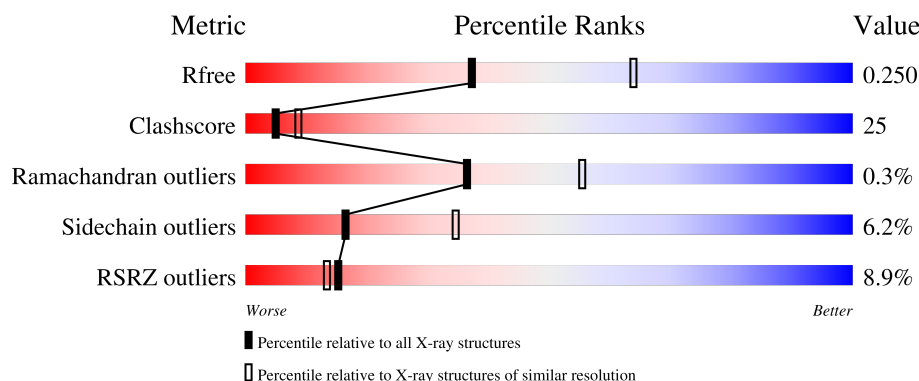
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	338	
1	B	338	

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	FLC	B	1471	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5071 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.

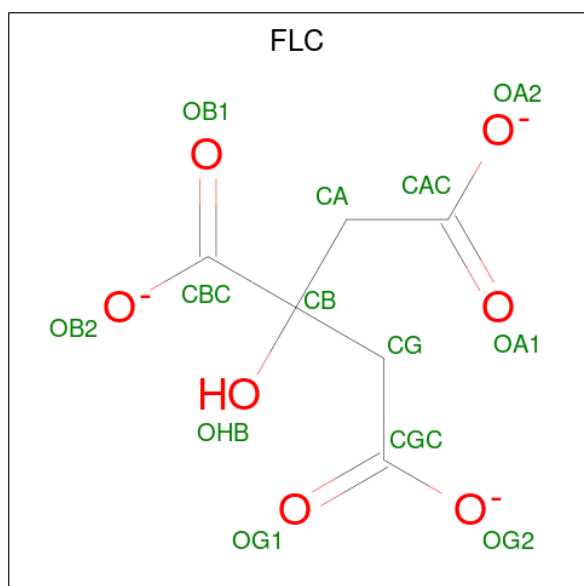
- Molecule 1 is a protein called REPLICATIVE DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2574	1616	456	491	11			
1	B	307	Total	C	N	O	S	0	0	0
			2353	1478	408	457	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ALA	-	expression tag	UNP O25916
B	151	ALA	-	expression tag	UNP O25916

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		
3	B	22	Total	O	0	0
			22	22		

i

● Molecule 1: REPLICATIVE DNA HELICASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.86Å 102.16Å 85.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.18 – 2.50 40.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.18-2.50) 98.6 (40.18-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.251 0.217 , 0.250	Depositor DCC
R_{free} test set	1547 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5071	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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](#)

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

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	0.40	0/2612	0.77	1/3511 (0.0%)
1	B	0.36	0/2382	0.80	3/3212 (0.1%)
All	All	0.39	0/4994	0.79	4/6723 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ARG	CA-C-N	7.35	127.35	119.78
1	B	366	ARG	C-N-CA	7.35	127.35	119.78
1	B	173	SER	N-CA-C	-6.11	102.42	110.43
1	A	472	HIS	N-CA-C	-5.22	103.25	110.35

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	2574	0	2586	81	0
1	B	2353	0	2279	172	0
2	A	13	0	5	0	0
2	B	26	0	10	9	0
3	A	83	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	0	1	0
All	All	5071	0	4880	247	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 25.

All (247) 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:359:LEU:CD1	1:B:362:ARG:HD3	1.24	1.56
1:B:359:LEU:HD12	1:B:362:ARG:CD	1.41	1.49
1:B:359:LEU:CD1	1:B:362:ARG:HH11	1.43	1.29
1:B:359:LEU:HD13	1:B:362:ARG:HH11	1.01	1.10
1:B:179:ILE:HD13	1:B:225:ARG:HD3	1.35	1.09
1:B:359:LEU:CD1	1:B:362:ARG:NH1	2.17	1.06
1:B:359:LEU:CD1	1:B:362:ARG:CD	2.14	1.03
1:B:467:MET:HG3	1:B:468:PRO:CD	1.89	1.03
1:B:467:MET:CG	1:B:468:PRO:HD3	1.91	1.00
1:B:467:MET:HG3	1:B:468:PRO:HD3	1.02	0.99
1:B:359:LEU:HD11	1:B:362:ARG:NH1	1.78	0.95
1:A:409:GLU:HG3	1:A:411:LYS:HZ3	1.32	0.94
1:B:207:MET:HE1	1:B:390:ARG:N	1.83	0.93
1:B:359:LEU:HD13	1:B:362:ARG:NH1	1.85	0.90
1:B:292:GLN:O	1:B:296:GLN:HG2	1.74	0.88
1:B:359:LEU:HD11	1:B:362:ARG:HH11	1.35	0.87
1:B:200:ILE:HD13	1:B:382:ALA:HB2	1.58	0.86
1:B:373:LYS:HG3	1:B:378:ILE:HG13	1.59	0.84
1:B:309:ILE:HG22	1:B:348:PRO:HD2	1.59	0.83
1:B:372:ILE:HG21	1:B:379:GLU:HB3	1.60	0.83
1:A:288:VAL:HG13	1:A:292:GLN:HB3	1.60	0.82
1:B:368:ILE:HG22	1:B:370:SER:H	1.45	0.82
1:A:409:GLU:HG3	1:A:411:LYS:NZ	1.95	0.81
1:B:194:ASN:C	1:B:348:PRO:HG3	2.05	0.80
1:B:174:LEU:O	1:B:174:LEU:HD23	1.83	0.78
1:A:447:ASN:N	2:B:1471:FLC:OG1	2.17	0.78
1:B:207:MET:HE1	1:B:390:ARG:H	1.46	0.76
1:B:234:MET:HE2	1:B:239:LEU:HD12	1.69	0.74
1:B:179:ILE:HD13	1:B:225:ARG:CD	2.16	0.74
1:A:246:ASP:HA	1:A:463:ARG:NH2	2.03	0.73
1:B:194:ASN:O	1:B:348:PRO:HG3	1.88	0.73
1:B:186:LEU:O	1:B:190:THR:HG22	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ALA:HB2	1:B:388:LEU:HB2	1.70	0.73
1:B:181:THR:HG21	1:B:186:LEU:HD23	1.69	0.73
1:B:221:LEU:HD21	1:B:278:LYS:CG	2.19	0.73
1:A:181:THR:HG21	1:A:186:LEU:HD23	1.71	0.72
1:B:175:GLU:HA	1:B:175:GLU:OE1	1.89	0.72
1:B:248:THR:HG21	1:B:268:LEU:HA	1.72	0.72
1:A:290:ILE:HD13	1:A:337:GLU:HB2	1.73	0.70
1:B:280:LEU:HD21	1:B:282:PHE:CE2	2.28	0.69
1:B:173:SER:O	1:B:174:LEU:HB3	1.92	0.69
1:B:200:ILE:HD13	1:B:382:ALA:CB	2.22	0.68
1:B:234:MET:HE3	1:B:238:GLN:HB3	1.74	0.68
1:A:291:GLU:HG2	1:A:294:ARG:HH21	1.57	0.68
1:B:239:LEU:HD22	1:B:282:PHE:HE1	1.59	0.67
1:B:209:LYS:HZ2	1:B:354:GLN:HE21	1.41	0.67
1:B:209:LYS:HG2	1:B:210:THR:N	2.07	0.67
1:A:309:ILE:HD11	1:A:350:ILE:HD13	1.78	0.66
1:B:221:LEU:HD21	1:B:278:LYS:HB3	1.77	0.66
1:A:246:ASP:HA	1:A:463:ARG:HH21	1.61	0.65
1:B:221:LEU:HD23	1:B:221:LEU:O	1.97	0.65
1:A:180:PRO:HD2	1:A:223:ASP:OD2	1.97	0.65
1:B:369:LEU:O	1:B:372:ILE:HB	1.97	0.65
1:A:468:PRO:HD2	1:A:471:SER:HB2	1.78	0.64
1:B:406:LEU:HD21	2:B:1471:FLC:HG1	1.78	0.64
1:B:208:GLY:HA2	2:B:1470:FLC:OG1	1.97	0.63
1:B:274:HIS:CE1	1:B:278:LYS:NZ	2.67	0.63
1:B:359:LEU:HD13	1:B:362:ARG:HD3	1.65	0.63
1:A:472:HIS:O	1:A:473:LEU:HB2	1.98	0.62
1:A:409:GLU:CG	1:A:411:LYS:HZ3	2.10	0.62
1:A:288:VAL:HG12	1:A:293:ILE:HG13	1.80	0.62
1:B:221:LEU:HD23	1:B:221:LEU:C	2.25	0.62
1:B:336:ARG:HA	1:B:381:ASP:OD2	1.99	0.61
1:A:308:GLY:O	1:A:348:PRO:HD2	2.00	0.61
1:B:447:ASN:N	1:B:447:ASN:HD22	1.99	0.61
1:A:467:MET:HG2	1:A:471:SER:HB2	1.81	0.60
1:B:153:ASN:HB3	1:B:156:GLU:HB3	1.83	0.60
1:A:241:LEU:HB3	1:A:252:MET:HE1	1.84	0.60
1:B:341:LEU:O	1:B:345:LEU:HG	2.01	0.60
1:B:221:LEU:HD21	1:B:278:LYS:CB	2.32	0.59
1:B:387:PHE:HB2	1:B:441:ILE:HB	1.84	0.59
1:B:209:LYS:HG3	1:B:352:LEU:HD23	1.85	0.59
1:B:210:THR:HB	2:B:1470:FLC:OG2	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LYS:HD2	3:A:2034:HOH:O	2.02	0.58
1:B:310:ALA:HB3	1:B:349:ILE:HD13	1.84	0.58
1:B:260:LEU:HB3	1:B:264:GLN:HB3	1.85	0.58
1:B:468:PRO:O	1:B:469:ILE:C	2.46	0.58
1:B:221:LEU:O	1:B:223:ASP:O	2.21	0.58
1:B:247:LEU:HD23	1:B:271:CYS:HB3	1.85	0.58
1:B:173:SER:O	1:B:174:LEU:CB	2.51	0.58
1:B:359:LEU:HD13	1:B:362:ARG:CD	2.26	0.57
1:B:185:GLN:O	1:B:189:TYR:HD1	1.88	0.57
1:B:179:ILE:CD1	1:B:225:ARG:HD3	2.21	0.57
1:B:274:HIS:NE2	1:B:278:LYS:NZ	2.52	0.57
1:B:368:ILE:HG22	1:B:370:SER:N	2.17	0.57
1:B:175:GLU:O	1:B:177:THR:HG23	2.05	0.56
1:B:359:LEU:CD1	1:B:362:ARG:CZ	2.82	0.56
1:B:466:ASP:HB3	3:B:2022:HOH:O	2.04	0.56
1:B:234:MET:HE2	1:B:239:LEU:CD1	2.34	0.56
1:B:204:ARG:NH1	1:B:205:PRO:HD3	2.22	0.55
1:B:237:GLU:O	1:B:240:ALA:N	2.39	0.55
1:B:421:LYS:O	1:B:425:GLU:HG3	2.06	0.55
1:A:472:HIS:O	1:A:473:LEU:CB	2.54	0.55
1:B:411:LYS:HZ3	2:B:1471:FLC:HA2	1.71	0.55
1:B:367:PRO:HB2	1:B:387:PHE:CG	2.42	0.55
1:B:310:ALA:HB3	1:B:349:ILE:CD1	2.37	0.54
1:B:345:LEU:O	1:B:346:GLU:HB2	2.07	0.54
1:B:359:LEU:O	1:B:360:GLU:C	2.51	0.54
1:A:469:ILE:O	1:A:472:HIS:O	2.26	0.54
1:A:261:ASP:C	1:A:261:ASP:OD1	2.51	0.54
1:A:458:ASN:OD1	1:A:460:PRO:HD2	2.07	0.54
1:B:221:LEU:HD21	1:B:278:LYS:HG3	1.90	0.54
1:B:209:LYS:NZ	1:B:354:GLN:HE21	2.07	0.53
1:B:316:GLN:HA	1:B:316:GLN:OE1	2.07	0.53
1:A:399:GLU:HG2	1:B:449:ALA:CB	2.37	0.53
1:A:227:VAL:HB	1:A:309:ILE:HG23	1.90	0.53
1:B:226:GLY:O	1:B:307:LEU:HD12	2.09	0.53
1:B:260:LEU:HB3	1:B:264:GLN:CB	2.37	0.53
1:A:174:LEU:HD11	1:B:425:GLU:HG2	1.91	0.53
1:B:161:ALA:O	1:B:165:ILE:HD13	2.09	0.52
1:A:181:THR:HG21	1:A:186:LEU:HB3	1.91	0.52
1:A:233:GLU:N	1:A:233:GLU:OE1	2.43	0.52
1:B:260:LEU:HB2	1:B:265:TRP:CD1	2.45	0.52
1:A:232:LEU:HB2	1:A:233:GLU:OE1	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASP:OD1	1:B:314:TYR:HB3	2.10	0.51
1:B:455:THR:HG21	1:B:464:TYR:HB3	1.90	0.51
1:A:223:ASP:CG	1:A:225:ARG:HE	2.18	0.51
1:B:314:TYR:HE1	1:B:316:GLN:CD	2.18	0.51
1:B:185:GLN:NE2	1:B:453:VAL:HG13	2.26	0.51
1:B:411:LYS:NZ	2:B:1471:FLC:HA2	2.25	0.51
1:B:372:ILE:CG2	1:B:379:GLU:HB3	2.37	0.51
1:B:259:ARG:C	1:B:260:LEU:HD23	2.36	0.50
1:B:309:ILE:HG22	1:B:348:PRO:CD	2.35	0.50
1:B:242:ARG:NH1	2:B:1470:FLC:OG2	2.43	0.50
1:B:392:TYR:OH	1:B:396:MET:HE3	2.11	0.50
1:B:221:LEU:C	1:B:221:LEU:CD2	2.85	0.50
1:B:190:THR:OG1	1:B:384:ILE:HD13	2.11	0.50
1:B:221:LEU:HD21	1:B:278:LYS:CD	2.41	0.50
1:B:291:GLU:O	1:B:295:LEU:HG	2.11	0.50
1:B:223:ASP:C	1:B:225:ARG:H	2.19	0.50
1:A:199:VAL:HB	1:A:350:ILE:HG13	1.94	0.50
1:A:436:GLU:HG3	1:A:457:PHE:HB3	1.93	0.50
1:B:459:ALA:HB3	1:B:460:PRO:HD3	1.93	0.50
1:A:408:LYS:O	1:A:409:GLU:HG2	2.11	0.49
1:B:167:GLU:HA	1:B:167:GLU:OE1	2.11	0.49
1:B:280:LEU:HD12	1:B:281:PHE:N	2.27	0.49
1:A:223:ASP:CG	1:A:225:ARG:HH21	2.20	0.49
1:B:228:ALA:O	1:B:310:ALA:HA	2.13	0.49
1:A:223:ASP:HB3	1:A:225:ARG:HG2	1.94	0.49
1:A:181:THR:HB	1:A:187:ASP:OD1	2.13	0.49
1:B:156:GLU:CD	1:B:156:GLU:O	2.56	0.49
1:A:446:ARG:HG2	2:B:1471:FLC:HA1	1.95	0.48
1:B:392:TYR:CZ	1:B:396:MET:HE3	2.48	0.48
1:B:252:MET:O	1:B:256:GLU:HG2	2.13	0.48
1:B:360:GLU:O	1:B:365:LYS:HE3	2.14	0.48
1:A:241:LEU:CB	1:A:252:MET:HE1	2.44	0.48
1:B:377:GLY:C	1:B:378:ILE:HD12	2.38	0.47
1:B:248:THR:HG22	1:B:271:CYS:SG	2.54	0.47
1:A:167:GLU:OE2	1:A:170:ARG:NH1	2.47	0.47
1:B:175:GLU:OE1	1:B:175:GLU:CA	2.61	0.47
1:B:311:PHE:CD1	1:B:350:ILE:HB	2.49	0.47
1:A:291:GLU:HG2	1:A:294:ARG:NH2	2.27	0.47
1:B:359:LEU:HD11	1:B:362:ARG:CZ	2.42	0.47
1:A:181:THR:CG2	1:A:186:LEU:HD23	2.41	0.47
1:A:467:MET:HG2	1:A:471:SER:CB	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LEU:HD22	1:B:282:PHE:CE1	2.46	0.47
1:B:378:ILE:HD12	1:B:378:ILE:N	2.30	0.47
1:B:221:LEU:CD2	1:B:278:LYS:HE2	2.45	0.47
1:B:314:TYR:HE1	1:B:316:GLN:OE1	1.99	0.46
1:B:158:LEU:O	1:B:162:MET:HG2	2.16	0.46
1:B:333:GLU:O	1:B:337:GLU:HG3	2.15	0.46
1:A:403:ILE:HD11	1:A:419:TYR:HA	1.97	0.46
1:B:385:VAL:C	1:B:386:LEU:HD23	2.41	0.46
1:A:251:ASN:ND2	1:A:253:HIS:HB3	2.31	0.46
1:B:272:PHE:C	1:B:272:PHE:CD1	2.93	0.45
1:B:380:GLN:O	1:B:444:LYS:NZ	2.49	0.45
1:B:365:LYS:HG2	1:B:394:TYR:CD1	2.52	0.45
1:B:367:PRO:HB2	1:B:387:PHE:CD1	2.51	0.45
1:A:369:LEU:HD13	1:A:443:ALA:HB1	1.99	0.45
1:A:212:LEU:CD2	1:A:388:LEU:HD11	2.47	0.45
1:A:294:ARG:HG3	1:A:341:LEU:HD13	1.99	0.45
1:A:205:PRO:O	1:A:206:SER:HB2	2.17	0.45
1:A:473:LEU:HD22	1:B:456:ARG:HG2	1.98	0.45
1:B:447:ASN:N	1:B:447:ASN:ND2	2.65	0.45
1:A:154:ILE:O	1:A:158:LEU:HG	2.17	0.45
1:A:185:GLN:NE2	1:A:469:ILE:HG12	2.31	0.45
1:B:446:ARG:C	1:B:447:ASN:HD22	2.25	0.45
1:A:288:VAL:HG13	1:A:292:GLN:CB	2.39	0.44
1:A:322:LYS:HB3	1:A:322:LYS:HE2	1.86	0.44
1:B:279:LYS:O	1:B:281:PHE:CE2	2.70	0.44
1:B:362:ARG:HH22	1:B:368:ILE:HG13	1.82	0.44
1:A:367:PRO:HB2	1:A:387:PHE:CG	2.52	0.44
1:A:404:ASP:O	1:A:405:LYS:C	2.60	0.44
1:A:395:GLN:O	1:A:399:GLU:HG3	2.18	0.44
1:A:446:ARG:HA	2:B:1471:FLC:OG1	2.17	0.44
1:B:333:GLU:O	1:B:336:ARG:HB3	2.18	0.44
1:B:359:LEU:HD12	1:B:362:ARG:CG	2.33	0.44
1:B:368:ILE:CG2	1:B:369:LEU:N	2.80	0.44
1:B:209:LYS:NZ	1:B:354:GLN:NE2	2.65	0.44
1:B:374:ASP:OD1	1:B:375:SER:N	2.51	0.44
1:B:223:ASP:C	1:B:225:ARG:N	2.76	0.43
1:B:355:LEU:CD1	1:B:367:PRO:HB3	2.47	0.43
1:A:330:GLN:HG2	3:A:2054:HOH:O	2.17	0.43
1:A:418:LEU:HD13	1:B:448:GLY:HA2	1.99	0.43
1:B:314:TYR:CE1	1:B:316:GLN:OE1	2.71	0.43
1:A:326:GLU:HB3	1:A:328:HIS:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:VAL:HB	1:B:350:ILE:HG13	2.00	0.43
1:B:181:THR:HG23	1:B:216:MET:HE2	2.00	0.43
1:B:378:ILE:O	1:B:380:GLN:OE1	2.37	0.43
1:A:180:PRO:CD	1:A:223:ASP:OD2	2.65	0.43
1:A:301:LYS:O	1:A:301:LYS:HD3	2.18	0.43
1:B:313:ASP:HA	1:B:314:TYR:HA	1.79	0.43
1:B:366:ARG:HA	1:B:367:PRO:HD3	1.71	0.43
1:B:373:LYS:HG3	1:B:378:ILE:CG1	2.41	0.42
1:A:468:PRO:HD2	1:A:471:SER:CB	2.49	0.42
1:B:350:ILE:HD12	1:B:350:ILE:N	2.34	0.42
1:A:399:GLU:HG2	1:B:449:ALA:HB2	2.00	0.42
1:A:467:MET:HA	1:A:468:PRO:HD3	1.90	0.42
1:B:457:PHE:CE1	1:B:459:ALA:HA	2.55	0.42
1:B:241:LEU:HD12	1:B:241:LEU:H	1.84	0.42
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.82	0.42
1:B:314:TYR:CD1	1:B:354:GLN:HG3	2.54	0.42
1:A:405:LYS:O	1:A:408:LYS:O	2.37	0.42
1:B:217:VAL:HG13	1:B:227:VAL:HG11	2.01	0.42
1:A:223:ASP:HB3	1:A:225:ARG:HE	1.84	0.42
1:B:164:LEU:HD12	1:B:164:LEU:O	2.19	0.42
1:B:259:ARG:O	1:B:260:LEU:HD23	2.20	0.42
1:B:359:LEU:HD12	1:B:362:ARG:HD3	0.45	0.42
1:A:290:ILE:CD1	1:A:337:GLU:HB2	2.44	0.41
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.92	0.41
1:B:171:LYS:C	1:B:173:SER:O	2.62	0.41
1:B:237:GLU:O	1:B:238:GLN:C	2.61	0.41
1:B:291:GLU:O	1:B:294:ARG:HB3	2.20	0.41
1:B:469:ILE:C	1:B:469:ILE:HD12	2.45	0.41
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.90	0.41
1:A:288:VAL:CG1	1:A:293:ILE:HG13	2.49	0.41
1:A:456:ARG:NH1	1:B:468:PRO:HG2	2.35	0.41
1:A:183:PHE:HB2	1:A:186:LEU:HB2	2.03	0.41
1:A:359:LEU:C	1:A:359:LEU:HD23	2.45	0.41
1:B:204:ARG:NH1	1:B:205:PRO:CD	2.82	0.41
1:B:204:ARG:HD2	1:B:355:LEU:HB2	2.03	0.41
1:B:294:ARG:NH2	1:B:337:GLU:OE1	2.54	0.41
1:A:374:ASP:O	1:A:375:SER:C	2.64	0.41
1:A:459:ALA:HB3	1:A:460:PRO:HD3	2.02	0.41
1:B:223:ASP:O	1:B:225:ARG:N	2.54	0.41
1:B:232:LEU:N	1:B:232:LEU:HD12	2.36	0.41
1:B:359:LEU:CD1	1:B:362:ARG:NE	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ARG:CZ	1:A:393:ILE:HD13	2.50	0.41
1:A:408:LYS:C	1:A:410:GLY:H	2.28	0.41
1:B:170:ARG:O	1:B:173:SER:O	2.39	0.41
1:B:236:ALA:O	1:B:237:GLU:C	2.63	0.41
1:B:379:GLU:C	1:B:379:GLU:CD	2.89	0.41
1:B:359:LEU:O	1:B:362:ARG:HG3	2.21	0.40
1:A:255:LEU:HA	1:A:260:LEU:HD21	2.04	0.40
1:A:419:TYR:CD1	1:A:419:TYR:C	2.98	0.40
1:B:176:VAL:C	1:B:177:THR:HG23	2.46	0.40
1:B:238:GLN:HA	1:B:241:LEU:HD13	2.02	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	322/338 (95%)	311 (97%)	11 (3%)	0	100	100
1	B	303/338 (90%)	288 (95%)	13 (4%)	2 (1%)	18	34
All	All	625/676 (92%)	599 (96%)	24 (4%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	ASP
1	B	467	MET

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	277/298 (93%)	262 (95%)	15 (5%)	20	41
1	B	241/298 (81%)	224 (93%)	17 (7%)	13	29
All	All	518/596 (87%)	486 (94%)	32 (6%)	16	34

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	GLU
1	A	165	ILE
1	A	227	VAL
1	A	239	LEU
1	A	295	LEU
1	A	301	LYS
1	A	306	GLU
1	A	356	ASN
1	A	359	LEU
1	A	369	LEU
1	A	388	LEU
1	A	393	ILE
1	A	409	GLU
1	A	450	THR
1	A	453	VAL
1	B	165	ILE
1	B	179	ILE
1	B	185	GLN
1	B	215	ASN
1	B	221	LEU
1	B	237	GLU
1	B	252	MET
1	B	275	LEU
1	B	309	ILE
1	B	338	LEU
1	B	356	ASN
1	B	368	ILE
1	B	383	ASP
1	B	393	ILE
1	B	412	ILE
1	B	447	ASN
1	B	455	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	215	ASN
1	A	303	GLN
1	A	328	HIS
1	A	354	GLN
1	A	361	ASN
1	A	401	ASN
1	A	423	ASN
1	B	188	ASN
1	B	215	ASN
1	B	222	ASN
1	B	354	GLN
1	B	361	ASN
1	B	401	ASN
1	B	431	GLN
1	B	447	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](#)

3 ligands are 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	FLC	B	1471	-	12,12,12	2.26	4 (33%)	17,17,17	1.62	3 (17%)
2	FLC	B	1470	-	12,12,12	2.11	4 (33%)	17,17,17	1.39	1 (5%)
2	FLC	A	1474	-	12,12,12	2.13	4 (33%)	17,17,17	1.32	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	B	1471	-	-	8/16/16/16	-
2	FLC	B	1470	-	-	5/16/16/16	-
2	FLC	A	1474	-	-	0/16/16/16	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1471	FLC	CB-CBC	-3.90	1.49	1.53
2	B	1471	FLC	CG-CB	-3.80	1.49	1.54
2	A	1474	FLC	CB-CBC	-3.73	1.49	1.53
2	B	1470	FLC	CB-CBC	-3.62	1.49	1.53
2	B	1470	FLC	CA-CB	-3.48	1.49	1.54
2	B	1471	FLC	CA-CB	-3.43	1.49	1.54
2	A	1474	FLC	CG-CB	-3.42	1.49	1.54
2	A	1474	FLC	CA-CB	-3.37	1.49	1.54
2	B	1470	FLC	CG-CB	-3.26	1.49	1.54
2	B	1471	FLC	OHB-CB	-3.09	1.37	1.43
2	A	1474	FLC	OHB-CB	-2.64	1.38	1.43
2	B	1470	FLC	OHB-CB	-2.60	1.38	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1471	FLC	OB2-CBC-CB	3.57	119.98	113.14
2	B	1470	FLC	OB2-CBC-CB	3.52	119.89	113.14
2	A	1474	FLC	OB2-CBC-CB	3.11	119.10	113.14
2	B	1471	FLC	OG2-CGC-CG	2.18	121.26	114.35
2	B	1471	FLC	CB-CA-CAC	2.11	119.69	113.92

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1471	FLC	CA-CB-CG-CGC
2	B	1471	FLC	OHB-CB-CG-CGC
2	B	1471	FLC	CBC-CB-CG-CGC
2	B	1471	FLC	CA-CB-CBC-OB1
2	B	1471	FLC	CA-CB-CBC-OB2
2	B	1471	FLC	CG-CB-CBC-OB2
2	B	1470	FLC	CAC-CA-CB-CBC
2	B	1470	FLC	CG-CB-CBC-OB1
2	B	1471	FLC	CG-CB-CBC-OB1
2	B	1470	FLC	CAC-CA-CB-CG
2	B	1470	FLC	OHB-CB-CBC-OB1
2	B	1471	FLC	OHB-CB-CBC-OB1
2	B	1470	FLC	CA-CB-CBC-OB1

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1471	FLC	6	0
2	B	1470	FLC	3	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	323/338 (95%)	0.14	13 (4%) 42 38	33, 55, 112, 142	1 (0%)
1	B	307/338 (90%)	1.04	43 (14%) 6 5	40, 107, 153, 172	0
All	All	630/676 (93%)	0.58	56 (8%) 15 13	33, 80, 145, 172	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	TYR	4.7
1	B	287	TYR	4.1
1	B	469	ILE	3.9
1	A	320	GLY	3.5
1	B	331	ILE	3.5
1	B	267	ASN	3.4
1	B	345	LEU	3.4
1	B	317	LEU	3.3
1	A	288	VAL	3.2
1	B	338	LEU	3.2
1	B	282	PHE	3.1
1	B	330	GLN	3.1
1	A	265[A]	TRP	3.0
1	A	467	MET	2.9
1	B	371	ASP	2.9
1	B	467	MET	2.9
1	B	378	ILE	2.9
1	A	154	ILE	2.8
1	B	231	SER	2.8
1	B	359	LEU	2.7
1	A	251	ASN	2.7
1	B	184	VAL	2.6
1	B	354	GLN	2.6
1	B	455	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	349	ILE	2.5
1	B	223	ASP	2.5
1	B	295	LEU	2.5
1	B	285	LYS	2.4
1	A	151	ALA	2.4
1	B	272	PHE	2.4
1	A	185	GLN	2.3
1	B	197	SER	2.3
1	B	246	ASP	2.3
1	B	230	PHE	2.3
1	B	185	GLN	2.3
1	A	470	ASP	2.3
1	B	176	VAL	2.3
1	B	307	LEU	2.3
1	B	353	VAL	2.3
1	A	260	LEU	2.2
1	B	280	LEU	2.2
1	B	297	LEU	2.2
1	B	178	GLY	2.2
1	B	302	SER	2.2
1	B	241	LEU	2.2
1	B	350	ILE	2.2
1	B	380	GLN	2.1
1	B	333	GLU	2.1
1	B	218	LEU	2.1
1	B	362	ARG	2.1
1	B	446	ARG	2.1
1	B	181	THR	2.1
1	B	303	GLN	2.0
1	A	473	LEU	2.0
1	B	154	ILE	2.0
1	A	319	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	FLC	B	1471	13/13	0.83	0.14	64,84,99,104	0
2	FLC	B	1470	13/13	0.86	0.16	94,113,117,117	0
2	FLC	A	1474	13/13	0.95	0.09	49,58,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.