Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:38 PM GMT

PDB ID	:	4A1F
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

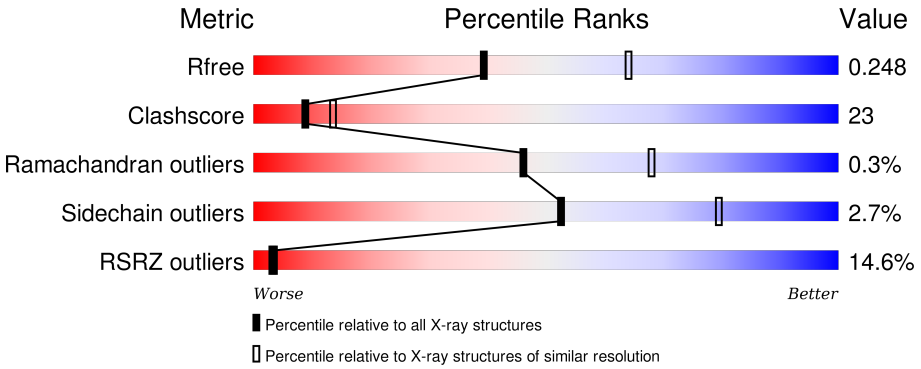
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	10% 72% 23%
1	B	338	17% 51% 38% 9%

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	X

2 Entry composition

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.

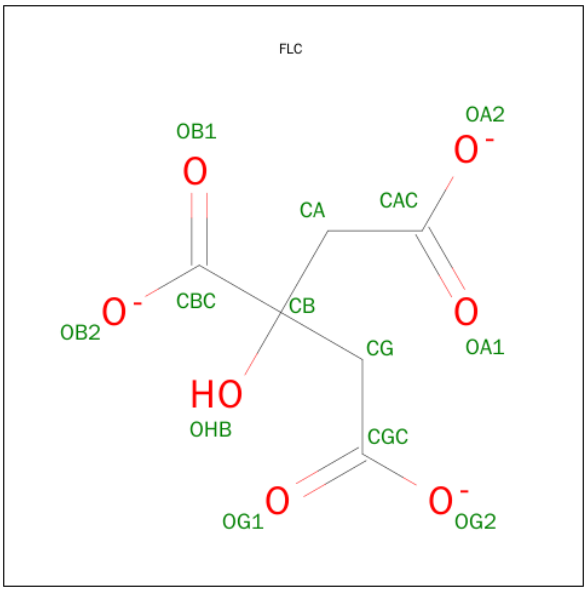
- Molecule 1 is a protein called REPLICATIVE DNA HELICASE.

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 (three-letter code: 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 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

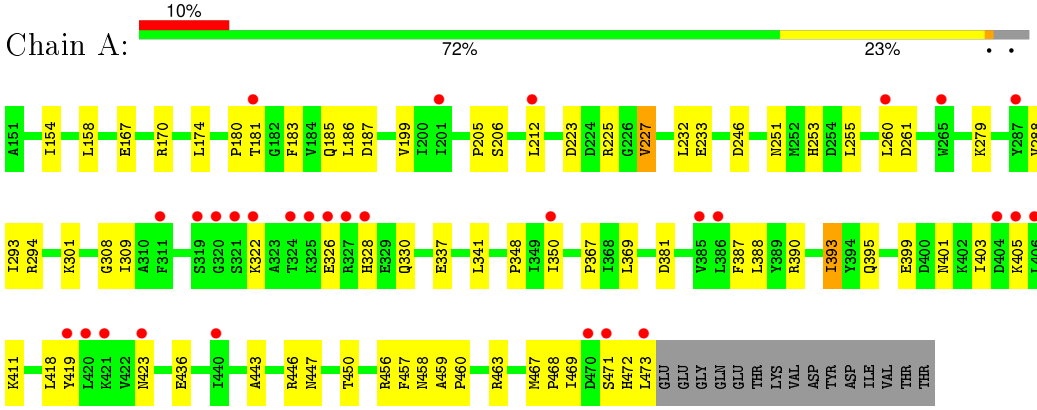
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	83	Total O 83 83	0	0
3	B	22	Total O 22 22	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

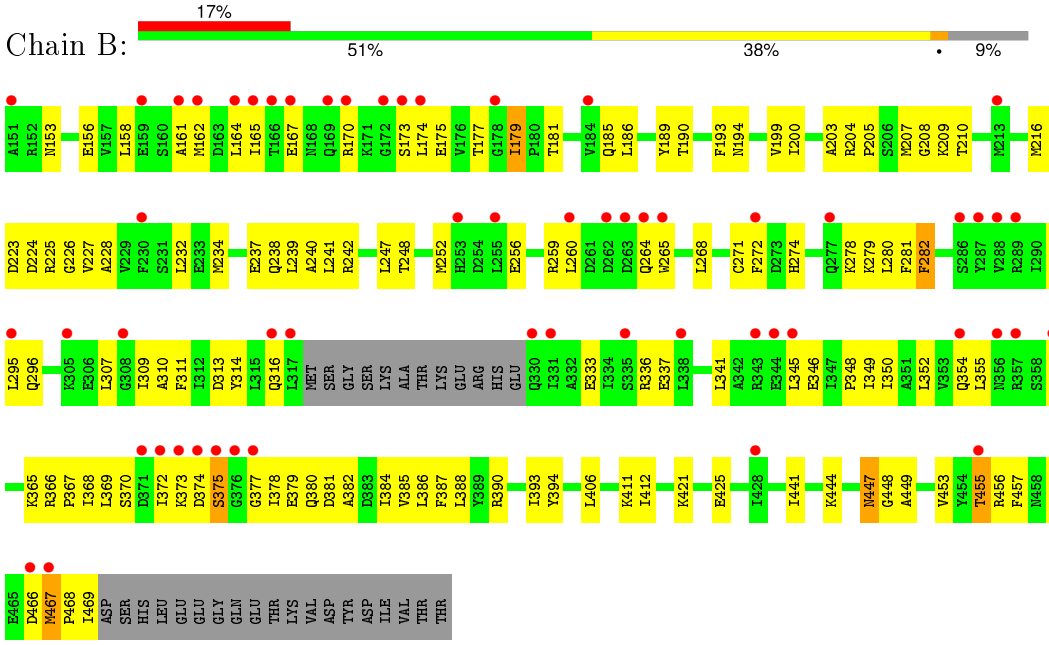
- Molecule 1: REPLICATIVE DNA HELICASE

Chain A:



- Molecule 1: REPLICATIVE DNA HELICASE

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.251 0.220 , 0.248	Depositor DCC
R_{free} test set	1547 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 64.4	EDS
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 30674 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.31	0/2612	0.47	0/3511
1	B	0.28	0/2382	0.47	0/3212
All	All	0.30	0/4994	0.47	0/6723

There are no bond length outliers.

There are no bond angle outliers.

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	2574	0	2586	74	0
1	B	2353	0	2279	162	0
2	A	13	0	5	0	0
2	B	26	0	10	9	0
3	A	83	0	0	2	0
3	B	22	0	0	1	0
All	All	5071	0	4880	230	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 23.

All (230) 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:207:MET:HE1	1:B:390:ARG:N	1.77	0.99
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:359:LEU:HD13	1:B:362:ARG:NH1	1.85	0.90
1:B:207:MET:HE1	1:B:390:ARG:H	1.34	0.89
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:174:LEU:HD23	1:B:174:LEU:O	1.83	0.78
1:A:447:ASN:N	2:B:1471:FLC:OG1	2.17	0.78
1:B:194:ASN:C	1:B:348:PRO:HG3	2.05	0.76
1:B:179:ILE:HD13	1:B:225:ARG:CD	2.16	0.74
1:B:194:ASN:O	1:B:348:PRO:HG3	1.88	0.74
1:A:246:ASP:HA	1:A:463:ARG:NH2	2.03	0.73
1:B:186:LEU:O	1:B:190:THR:HG22	1.88	0.73
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:B:175:GLU:OE1	1:B:175:GLU:HA	1.89	0.73
1:A:181:THR:HG21	1:A:186:LEU:HD23	1.71	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:234:MET:HE2	1:B:239:LEU:HD12	1.72	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:HD13	1:B:382:ALA:CB	2.22	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:HG2	1:B:210:THR:N	2.07	0.67
1:B:221:LEU:HD21	1:B:278:LYS:HB3	1.77	0.66
1:A:309:ILE:HD11	1:A:350:ILE:HD13	1.78	0.66
1:A:246:ASP:HA	1:A:463:ARG:HH21	1.61	0.65
1:B:221:LEU:O	1:B:221:LEU:HD23	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:B:406:LEU:HD21	2:B:1471:FLC:HG1	1.78	0.64
1:A:468:PRO:HD2	1:A:471:SER:HB2	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: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: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
1:B:310:ALA:HB3	1:B:349:ILE:HD13	1.84	0.58
1:A:279:LYS:HD2	3:A:2034:HOH:O	2.02	0.58
1:B:260:LEU:HB3	1:B:264:GLN:HB3	1.85	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:209:LYS:HZ2	1:B:354:GLN:HE21	1.53	0.57
1:B:359:LEU:HD13	1:B:362:ARG:CD	2.26	0.57
1:B:221:LEU:C	1:B:221:LEU:HD23	2.25	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:368:ILE:HG22	1:B:370:SER:N	2.17	0.57
1:B:274:HIS:NE2	1:B:278:LYS:NZ	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:469:ILE:O	1:A:472:HIS:O	2.26	0.54
1:B:221:LEU:HD21	1:B:278:LYS:HG3	1.90	0.54
1:A:458:ASN:OD1	1:A:460:PRO:HD2	2.07	0.54
1:B:468:PRO:O	1:B:469:ILE:C	2.46	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:260:LEU:HB3	1:B:264:GLN:CB	2.37	0.53
1:B:226:GLY:O	1:B:307:LEU:HD12	2.09	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:OE1	1:A:233:GLU:N	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
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: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: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: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: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:B:359:LEU:O	1:B:360:GLU:C	2.51	0.49
1:A:408:LYS:O	1:A:409:GLU:HG2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD12	1:B:281:PHE:N	2.27	0.49
1:B:167:GLU:OE1	1:B:167:GLU:HA	2.11	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:261:ASP:C	1:A:261:ASP:OD1	2.51	0.49
1:A:181:THR:HB	1:A:187:ASP:OD1	2.13	0.49
1:A:446:ARG:HG2	2:B:1471:FLC:HA1	1.95	0.48
1:B:360:GLU:O	1:B:365:LYS:HE3	2.14	0.48
1:B:252:MET:O	1:B:256:GLU:HG2	2.13	0.48
1:B:248:THR:HG22	1:B:271:CYS:SG	2.54	0.47
1:B:175:GLU:OE1	1:B:175:GLU:CA	2.61	0.47
1:A:167:GLU:OE2	1:A:170:ARG:NH1	2.47	0.47
1:B:311:PHE:CD1	1:B:350:ILE:HB	2.49	0.47
1:B:359:LEU:HD11	1:B:362:ARG:CZ	2.42	0.47
1:A:291:GLU:HG2	1:A:294:ARG:NH2	2.27	0.47
1:B:378:ILE:HD12	1:B:378:ILE:N	2.30	0.47
1:A:181:THR:CG2	1:A:186:LEU:HD23	2.41	0.47
1:B:239:LEU:HD22	1:B:282:PHE:CE1	2.46	0.47
1:A:467:MET:HG2	1:A:471:SER:CB	2.45	0.47
1:B:221:LEU:CD2	1:B:278:LYS:HE2	2.45	0.47
1:A:223:ASP:CG	1:A:225:ARG:HE	2.18	0.47
1:B:314:TYR:HE1	1:B:316:GLN:CD	2.18	0.46
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:B:193:PHE:HZ	1:B:216:MET:HE1	1.81	0.46
1:B:259:ARG:C	1:B:260:LEU:HD23	2.36	0.46
1:A:403:ILE:HD11	1:A:419:TYR:HA	1.97	0.46
1:A:251:ASN:ND2	1:A:253:HIS:HB3	2.31	0.46
1:B:221:LEU:C	1:B:221:LEU:CD2	2.85	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:223:ASP:C	1:B:225:ARG:H	2.19	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:294:ARG:HG3	1:A:341:LEU:HD13	1.99	0.45
1:A:212:LEU:CD2	1:A:388:LEU:HD11	2.47	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:205:PRO:O	1:A:206:SER:HB2	2.17	0.45
1:A:154:ILE:O	1:A:158:LEU:HG	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:NE2	1:A:469:ILE:HG12	2.31	0.45
1:B:207:MET:HE3	1:B:390:ARG:HG3	1.97	0.44
1:A:288:VAL:HG13	1:A:292:GLN:CB	2.39	0.44
1:A:223:ASP:CG	1:A:225:ARG:HH21	2.20	0.44
1:A:322:LYS:HE2	1:A:322:LYS:HB3	1.86	0.44
1:B:362:ARG:HH22	1:B:368:ILE:HG13	1.82	0.44
1:B:279:LYS:O	1:B:281:PHE:CE2	2.70	0.44
1:A:367:PRO:HB2	1:A:387:PHE:CG	2.52	0.44
1:A:446:ARG:HA	2:B:1471:FLC:OG1	2.17	0.44
1:A:395:GLN:O	1:A:399:GLU:HG3	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:333:GLU:O	1:B:336:ARG:HB3	2.18	0.44
1:B:156:GLU:O	1:B:156:GLU:CD	2.56	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: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:B:411:LYS:HZ2	2:B:1471:FLC:HA2	1.84	0.43
1:A:326:GLU:HB3	1:A:328:HIS:HD2	1.84	0.43
1:B:377:GLY:C	1:B:378:ILE:HD12	2.38	0.43
1:B:199:VAL:HB	1:B:350:ILE:HG13	2.00	0.43
1:B:378:ILE:O	1:B:380:GLN:OE1	2.37	0.43
1:B:313:ASP:HA	1:B:314:TYR:HA	1.79	0.43
1:A:180:PRO:CD	1:A:223:ASP:OD2	2.65	0.43
1:B:366:ARG:HA	1:B:367:PRO:HD3	1.71	0.43
1:A:301:LYS:O	1:A:301:LYS:HD3	2.18	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:N	1:B:350:ILE:HD12	2.34	0.42
1:A:467:MET:HA	1:A:468:PRO:HD3	1.90	0.42
1:A:399:GLU:HG2	1:B:449:ALA:HB2	2.00	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:B:234:MET:HE3	1:B:242:ARG:NH2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:HB3	1:A:225:ARG:HE	1.84	0.42
1:B:359:LEU:HD12	1:B:362:ARG:HD3	0.45	0.42
1:B:259:ARG:O	1:B:260:LEU:HD23	2.20	0.42
1:B:164:LEU:HD12	1:B:164:LEU:O	2.19	0.42
1:A:290:ILE:CD1	1:A:337:GLU:HB2	2.44	0.41
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.92	0.41
1:B:291:GLU:O	1:B:294:ARG:HB3	2.20	0.41
1:A:456:ARG:NH1	1:B:468:PRO:HG2	2.35	0.41
1:A:288:VAL:CG1	1:A:293:ILE:HG13	2.49	0.41
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.90	0.41
1:A:183:PHE:HB2	1:A:186:LEU:HB2	2.03	0.41
1:B:204:ARG:NH1	1:B:205:PRO:CD	2.82	0.41
1:B:385:VAL:C	1:B:386:LEU:HD23	2.41	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:B:359:LEU:CD1	1:B:362:ARG:NE	2.79	0.41
1:B:223:ASP:O	1:B:225:ARG:N	2.54	0.41
1:A:459:ALA:HB3	1:A:460:PRO:HD3	2.02	0.41
1:B:272:PHE:CD1	1:B:272:PHE:C	2.93	0.41
1:B:232:LEU:HD12	1:B:232:LEU:N	2.36	0.41
1:B:170:ARG:O	1:B:173:SER:O	2.39	0.41
1:A:390:ARG:CZ	1:A:393:ILE:HD13	2.50	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: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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	303/338 (90%)	288 (95%)	13 (4%)	2 (1%)	26 46
All	All	625/676 (92%)	599 (96%)	24 (4%)	2 (0%)	46 68

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%)	271 (98%)	6 (2%)	60 84
1	B	241/298 (81%)	233 (97%)	8 (3%)	45 73
All	All	518/596 (87%)	504 (97%)	14 (3%)	52 79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	VAL
1	A	381	ASP
1	A	393	ILE
1	A	401	ASN
1	A	423	ASN
1	A	450	THR
1	B	179	ILE
1	B	221	LEU
1	B	282	PHE
1	B	375	SER
1	B	393	ILE
1	B	412	ILE
1	B	447	ASN
1	B	455	THR

Some 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	A	472	HIS
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	447	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	1474	-	3,12,12	3.17	3 (100%)	3,17,17	1.53	1 (33%)
2	FLC	B	1470	-	3,12,12	3.15	3 (100%)	3,17,17	1.50	1 (33%)
2	FLC	B	1471	-	3,12,12	3.47	3 (100%)	3,17,17	2.15	2 (66%)

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	A	1474	-	-	0/6/16/16	0/0/0/0
2	FLC	B	1470	-	-	0/6/16/16	0/0/0/0
2	FLC	B	1471	-	-	0/6/16/16	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1471	FLC	CG-CB	-3.59	1.49	1.54
2	B	1471	FLC	OHB-CB	-3.51	1.37	1.43
2	B	1470	FLC	CA-CB	-3.33	1.49	1.54
2	B	1471	FLC	CA-CB	-3.29	1.49	1.54
2	A	1474	FLC	CG-CB	-3.28	1.49	1.54
2	A	1474	FLC	CA-CB	-3.24	1.49	1.54
2	B	1470	FLC	CG-CB	-3.15	1.49	1.54
2	A	1474	FLC	OHB-CB	-2.99	1.38	1.43
2	B	1470	FLC	OHB-CB	-2.95	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1474	FLC	CB-CG-CGC	2.17	118.42	114.96
2	B	1471	FLC	CB-CG-CGC	2.22	118.50	114.96
2	B	1470	FLC	CB-CG-CGC	2.24	118.54	114.96
2	B	1471	FLC	CB-CA-CAC	2.96	119.69	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1470	FLC	3	0
2	B	1471	FLC	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, 95^{th} 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%)	0.64	34 (10%)	8	8	33, 55, 112, 142	0
1	B	307/338 (90%)	1.02	58 (18%)	2	1	40, 107, 153, 172	0
All	All	630/676 (93%)	0.83	92 (14%)	3	3	33, 80, 145, 172	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	ILE	7.5
1	A	287	TYR	7.3
1	B	287	TYR	6.9
1	B	371	ASP	4.9
1	A	320	GLY	4.8
1	B	338	LEU	4.6
1	B	262	ASP	4.6
1	B	151	ALA	4.6
1	B	260	LEU	4.4
1	B	376	GLY	4.2
1	A	319	SER	4.2
1	B	375	SER	4.2
1	B	317	LEU	4.1
1	B	374	ASP	4.0
1	A	410	GLY	3.9
1	B	467	MET	3.8
1	B	345	LEU	3.5
1	B	169	GLN	3.5
1	A	260	LEU	3.4
1	B	265	TRP	3.3
1	B	272	PHE	3.3
1	A	406	LEU	3.3
1	A	470	ASP	3.2
1	B	357	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	170	ARG	3.2
1	A	328	HIS	3.2
1	A	409	GLU	3.2
1	B	263	ASP	3.2
1	A	404	ASP	3.1
1	B	372	ILE	3.1
1	A	471	SER	3.1
1	B	164	LEU	3.0
1	B	335	SER	3.0
1	B	377	GLY	2.9
1	A	326	GLU	2.9
1	A	324	THR	2.8
1	B	166	THR	2.8
1	A	350	ILE	2.8
1	A	440	ILE	2.8
1	B	230	PHE	2.8
1	A	201	ILE	2.8
1	A	408	LYS	2.8
1	A	385	VAL	2.8
1	B	343	ARG	2.7
1	B	165	ILE	2.7
1	B	277	GLN	2.7
1	A	423	ASN	2.7
1	A	327	ARG	2.7
1	B	373	LYS	2.7
1	B	255	LEU	2.7
1	A	419	TYR	2.7
1	A	321	SER	2.6
1	B	288	VAL	2.6
1	B	174	LEU	2.6
1	B	428	ILE	2.6
1	A	420	LEU	2.6
1	B	161	ALA	2.5
1	B	308	GLY	2.5
1	B	356	ASN	2.5
1	A	407	LYS	2.5
1	B	264	GLN	2.5
1	B	172	GLY	2.5
1	B	289	ARG	2.4
1	B	184	VAL	2.4
1	B	162	MET	2.4
1	B	305	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	253	HIS	2.4
1	B	159	GLU	2.4
1	A	473	LEU	2.4
1	B	362	ARG	2.3
1	B	466	ASP	2.3
1	A	181	THR	2.3
1	B	178	GLY	2.3
1	B	213	MET	2.3
1	A	421	LYS	2.3
1	B	330	GLN	2.2
1	A	322	LYS	2.2
1	B	173	SER	2.2
1	A	386	LEU	2.2
1	A	265[A]	TRP	2.2
1	B	359	LEU	2.2
1	B	455	THR	2.2
1	B	167	GLU	2.2
1	B	344	GLU	2.1
1	B	316	GLN	2.1
1	A	325	LYS	2.1
1	B	295	LEU	2.1
1	A	311	PHE	2.1
1	A	405	LYS	2.1
1	A	212	LEU	2.0
1	B	354	GLN	2.0
1	B	286	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	FLC	B	1471	13/13	0.79	0.24	2.70	64,84,99,104	0
2	FLC	B	1470	13/13	0.87	0.14	-0.38	94,113,117,117	0
2	FLC	A	1474	13/13	0.96	0.15	-0.75	49,58,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.