Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:39 PM GMT

PDB ID	:	1LB2
Title	:	Structure of the E. coli alpha C-terminal domain of RNA polymerase in complex with CAP and DNA
Authors	:	Benoff, B.; Yang, H.; Lawson, C.L.; Parkinson, G.; Liu, J.; Blatter, E.; Ebright, Y.W.; Berman, H.M.; Ebright, R.H.
Deposited on	:	2002-04-01
Resolution	:	3.10 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:

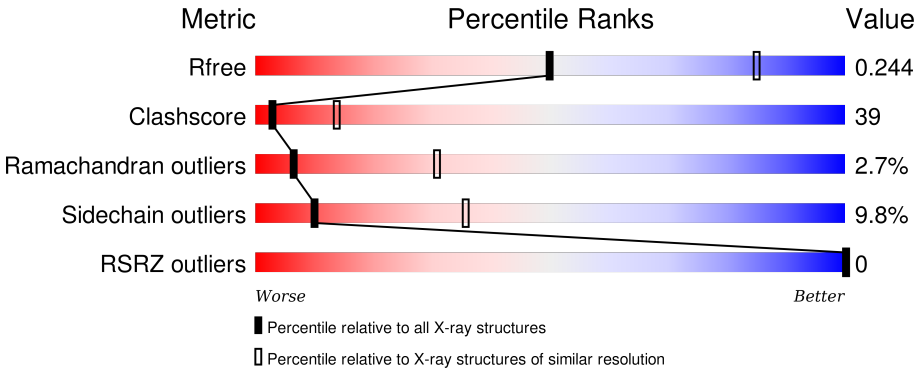
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	K	20	40% 50% 10%
2	J	24	58% 42%
3	A	209	47% 45%
4	B	84	20% 56% 8% 14%
4	E	84	27% 39% 11% 21%

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
5	CMP	A	679	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3613 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 DNA chain called 5'-D(*CP*TP*TP*TP*TP*TP*TP*CP*CP*TP*AP*AP *AP*AP*TP*GP*TP*GP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	20	Total	C	N	O	P	0	0	0
			403	197	64	123	19			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*GP*AP*TP*CP*AP*CP*AP*TP*TP *TP*TP*AP*GP*GP*AP*AP*AP*AP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	24	Total	C	N	O	P	0	0	0
			493	237	96	137	23			

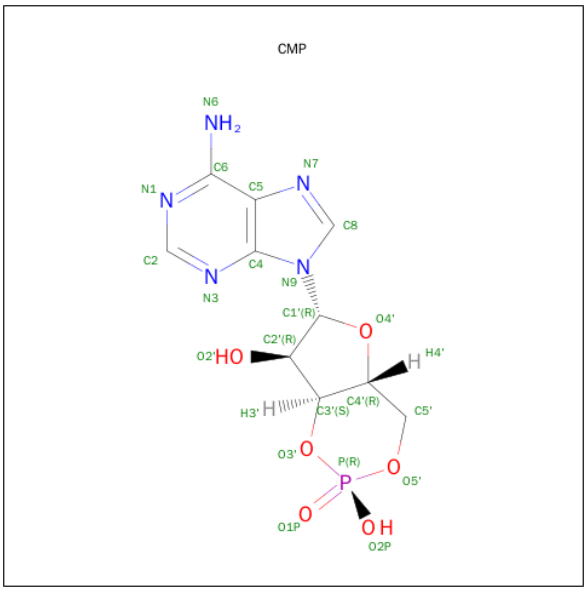
- Molecule 3 is a protein called CATABOLITE GENE ACTIVATOR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	201	Total	C	N	O	S	0	0	0
			1591	1007	280	295	9			

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	72	Total	C	N	O	S	0	0	0
			565	357	99	107	2			
4	E	66	Total	C	N	O	S	0	0	0
			507	320	88	98	1			

- Molecule 5 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 6 is water.

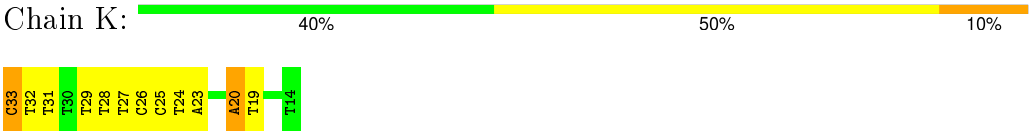
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total	O	0	0
			1	1		
6	J	6	Total	O	0	0
			6	6		
6	A	19	Total	O	0	0
			19	19		
6	B	4	Total	O	0	0
			4	4		
6	E	2	Total	O	0	0
			2	2		

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: 5'-D(*CP*TP*TP*TP*TP*TP*TP*CP*CP*TP*AP*AP*AP*AP*TP*GP*TP*GP*AP*T)-3'

Chain K:

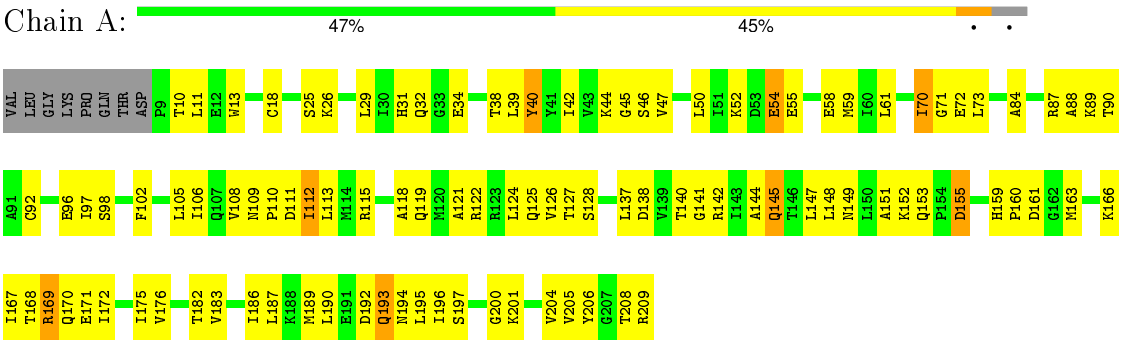


• Molecule 2: 5'-D(*CP*TP*AP*GP*AP*TP*CP*AP*CP*AP*TP*TP*TP*TP*AP*GP*GP*AP*AP*AP*AP*AP*AP*G)-3'

Chain J:

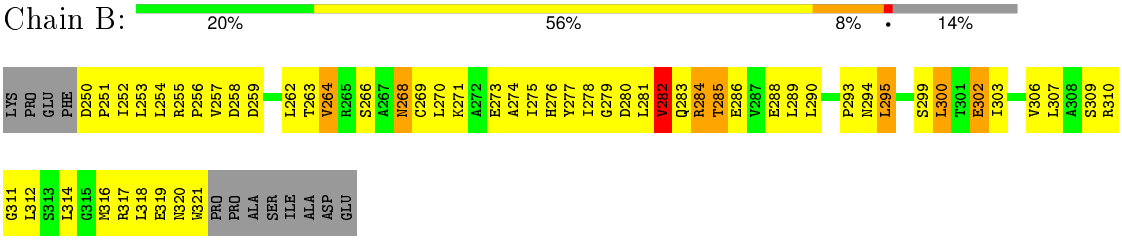
• Molecule 3: CATABOLITE GENE ACTIVATOR PROTEIN

Chain A:



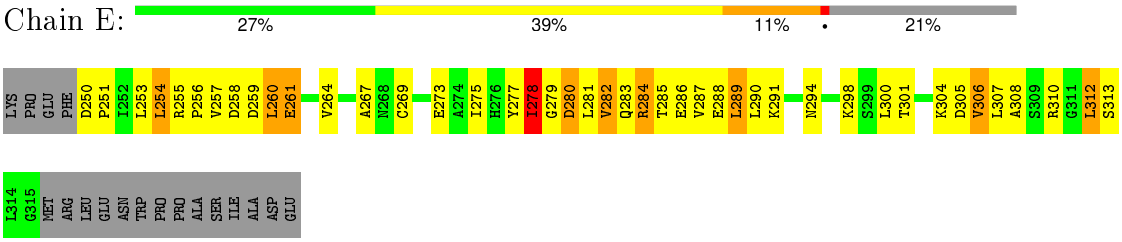
• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain B:



• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain E:


27%
39%
11%
21%
LYS PRO GLU PHE D250 P251 I252 L253 L254 R255 P256 V257 D258 D259 L260 E261 V264 A267 N268 C269 E273 A274 I275 H276 Y277 I278 G279 D280 L281 V282 Q283 R284 T285 E286 V287 E288 L289 L290 K291 N294 K298 S299 L300 T301 K304 D305 V306 L307 A308 S309 R310 G311 L312 S313
L314 G315 MET ARG LEU GLU ASN TRP PRO PRO PRO ALA SER ILE ALA ASP GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	175.97Å 175.97Å 158.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.03 – 3.10	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-3.10) 88.0 (20.03-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 3.09Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.244 0.216 , 0.244	Depositor DCC
R_{free} test set	2304 reflections (9.88%)	DCC
Wilson B-factor (Å^2)	102.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 69.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 23331 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3613	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: CMP

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	K	0.57	0/449	0.75	0/691
2	J	0.61	0/555	0.77	0/855
3	A	0.51	0/1616	0.75	0/2174
4	B	0.36	0/571	0.66	0/772
4	E	0.34	0/511	0.65	0/691
All	All	0.49	0/3702	0.73	0/5183

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	20	DA	Sidechain
1	K	33	DC	Sidechain

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	K	403	0	232	16	0
2	J	493	0	272	14	0
3	A	1591	0	1632	101	0
4	B	565	0	595	76	0
4	E	507	0	540	72	0
5	A	22	0	11	7	0
6	A	19	0	0	1	0
6	B	4	0	0	1	0
6	E	2	0	0	0	0
6	J	6	0	0	0	0
6	K	1	0	0	0	0
All	All	3613	0	3282	270	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 39.

All (270) 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)
5:A:679:CMP:H2	5:A:679:CMP:C2	0.97	1.50
4:B:282:VAL:HG22	4:B:316:MET:HG3	1.35	1.09
4:E:255:ARG:HE	4:E:256:PRO:HD2	1.15	1.08
4:B:285:THR:HG23	4:B:288:GLU:HG2	1.26	1.07
4:B:264:VAL:HG12	4:B:268:ASN:HD21	1.13	1.05
4:E:256:PRO:HA	4:E:277:TYR:HA	1.50	0.91
3:A:73:LEU:HD12	5:A:679:CMP:H3'	1.54	0.90
3:A:45:GLY:HA3	3:A:92:CYS:HB3	1.56	0.88
4:E:285:THR:H	4:E:288:GLU:HG3	1.40	0.87
2:J:14:DA:H2"	2:J:15:DT:H5'	1.55	0.86
4:E:255:ARG:NE	4:E:256:PRO:HD2	1.90	0.86
4:B:285:THR:CG2	4:B:288:GLU:HG2	2.04	0.85
4:B:279:GLY:HA3	4:B:321:TRP:CZ2	2.11	0.85
4:E:290:LEU:HD21	4:E:300:LEU:HD22	1.58	0.85
4:E:310:ARG:O	4:E:312:LEU:HD12	1.81	0.80
4:E:307:LEU:HA	4:E:310:ARG:HB2	1.64	0.79
1:K:33:DC:H2'	1:K:32:DT:H72	1.63	0.79
4:B:250:ASP:CG	4:B:251:PRO:HD2	2.04	0.78
4:E:253:LEU:HD23	4:E:253:LEU:O	1.84	0.78
4:B:264:VAL:HG12	4:B:268:ASN:ND2	1.96	0.78
4:B:295:LEU:HD23	4:B:299:SER:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:282:VAL:HG21	4:B:312:LEU:HD23	1.66	0.76
4:E:282:VAL:HG13	4:E:313:SER:O	1.86	0.76
4:E:284:ARG:HB3	4:E:284:ARG:NH1	2.00	0.76
4:B:253:LEU:HD12	4:B:253:LEU:H	1.50	0.75
4:B:278:ILE:O	4:B:282:VAL:HB	1.85	0.74
4:E:285:THR:H	4:E:288:GLU:CG	1.99	0.74
3:A:31:HIS:HB3	3:A:34:GLU:OE1	1.87	0.74
4:E:306:VAL:HG23	4:E:307:LEU:HD13	1.70	0.73
4:E:257:VAL:O	4:E:260:LEU:HB2	1.88	0.73
4:B:279:GLY:HA3	4:B:321:TRP:CH2	2.24	0.72
1:K:29:DT:H2"	1:K:28:DT:H5'	1.72	0.72
1:K:20:DA:H2'	3:A:170:GLN:HE21	1.54	0.72
3:A:126:VAL:HG23	3:A:127:THR:N	2.05	0.71
3:A:45:GLY:HA3	3:A:92:CYS:CB	2.20	0.71
4:E:278:ILE:O	4:E:278:ILE:HD12	1.89	0.71
4:E:289:LEU:HD12	4:E:289:LEU:H	1.54	0.70
3:A:54:GLU:HG2	3:A:55:GLU:OE2	1.90	0.70
2:J:30:DA:H5"	4:E:294:ASN:ND2	2.06	0.70
3:A:13:TRP:CZ2	3:A:105:LEU:HD23	2.26	0.70
4:E:307:LEU:HB3	4:E:312:LEU:O	1.93	0.69
3:A:105:LEU:O	3:A:108:VAL:HG22	1.93	0.69
4:B:282:VAL:HG22	4:B:316:MET:CG	2.18	0.69
4:E:253:LEU:HA	4:E:278:ILE:HG13	1.75	0.69
4:B:289:LEU:HD12	4:B:314:LEU:HD21	1.76	0.68
4:B:285:THR:HG23	4:B:288:GLU:CG	2.13	0.68
3:A:44:LYS:O	3:A:92:CYS:HB2	1.93	0.68
2:J:30:DA:H5"	4:E:294:ASN:HD22	1.59	0.68
3:A:182:THR:O	3:A:186:ILE:HD13	1.93	0.68
3:A:172:ILE:O	3:A:176:VAL:HG22	1.94	0.67
4:E:284:ARG:HB3	4:E:284:ARG:HH11	1.59	0.67
4:B:262:LEU:HD13	4:B:266:SER:HB2	1.77	0.67
3:A:189:MET:HG2	3:A:193:GLN:HE21	1.60	0.66
4:B:252:ILE:HA	4:B:255:ARG:HH12	1.61	0.66
3:A:192:ASP:C	3:A:194:ASN:H	2.00	0.65
4:B:257:VAL:HA	4:B:278:ILE:HG22	1.77	0.64
4:B:252:ILE:HA	4:B:255:ARG:NH1	2.12	0.64
4:E:282:VAL:HG21	4:E:312:LEU:HD22	1.79	0.64
3:A:97:ILE:HG22	3:A:98:SER:O	1.98	0.64
3:A:102:PHE:O	3:A:106:ILE:HG13	1.99	0.63
4:E:251:PRO:HA	4:E:254:LEU:HD22	1.79	0.63
4:B:263:THR:HG22	4:B:302:GLU:OE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:282:VAL:HG21	4:E:312:LEU:CD2	2.28	0.62
4:B:263:THR:HG23	4:B:266:SER:H	1.65	0.62
4:E:279:GLY:O	4:E:283:GLN:HG3	1.99	0.62
4:E:257:VAL:HG23	4:E:258:ASP:N	2.14	0.62
4:B:312:LEU:HD12	4:B:312:LEU:N	2.14	0.61
4:E:286:GLU:HG2	4:E:300:LEU:HD11	1.81	0.61
3:A:31:HIS:HB3	3:A:34:GLU:CD	2.21	0.61
3:A:54:GLU:CD	3:A:54:GLU:H	2.04	0.61
4:B:266:SER:O	4:B:270:LEU:HD12	2.00	0.61
4:B:282:VAL:CG2	4:B:316:MET:HG3	2.23	0.61
2:J:14:DA:C2'	2:J:15:DT:H5'	2.29	0.60
4:B:270:LEU:CD2	4:B:281:LEU:HD13	2.31	0.60
4:E:285:THR:OG1	4:E:288:GLU:HG2	2.02	0.60
3:A:205:VAL:O	3:A:205:VAL:HG23	2.02	0.60
4:B:253:LEU:HA	4:B:278:ILE:HG13	1.82	0.60
4:B:284:ARG:O	4:B:314:LEU:HG	2.02	0.59
3:A:167:ILE:HD13	3:A:172:ILE:HG12	1.85	0.59
3:A:189:MET:HG2	3:A:193:GLN:NE2	2.17	0.59
4:B:253:LEU:HB3	4:B:321:TRP:CH2	2.37	0.58
1:K:33:DC:H2'	1:K:32:DT:C7	2.30	0.58
3:A:10:THR:O	3:A:13:TRP:HB3	2.03	0.58
3:A:145:GLN:O	3:A:148:LEU:HB2	2.02	0.58
4:E:301:THR:HA	4:E:304:LYS:CE	2.34	0.58
1:K:20:DA:H2'	3:A:170:GLN:NE2	2.17	0.58
3:A:18:CYS:SG	3:A:97:ILE:HG13	2.43	0.58
4:E:251:PRO:O	4:E:254:LEU:HD22	2.04	0.58
4:B:318:LEU:HD12	4:B:318:LEU:O	2.04	0.58
4:E:253:LEU:HG	4:E:279:GLY:HA2	1.86	0.58
3:A:25:SER:O	3:A:26:LYS:HB2	2.03	0.58
4:B:253:LEU:HA	4:B:278:ILE:CD1	2.34	0.57
4:E:250:ASP:CG	4:E:251:PRO:HD2	2.25	0.57
3:A:71:GLY:HA2	5:A:679:CMP:P	2.44	0.57
2:J:32:DA:P	4:E:264:VAL:HG21	2.45	0.57
3:A:209:ARG:HB3	4:B:317:ARG:HD2	1.85	0.57
3:A:50:LEU:C	3:A:50:LEU:HD12	2.24	0.57
1:K:25:DC:H2"	1:K:24:DT:H71	1.87	0.57
3:A:87:ARG:HH11	3:A:87:ARG:HG3	1.70	0.57
4:B:253:LEU:HA	4:B:278:ILE:HD11	1.87	0.56
3:A:172:ILE:HA	3:A:175:ILE:HG13	1.88	0.56
2:J:13:DG:OP1	3:A:138:ASP:HB2	2.05	0.56
4:B:270:LEU:HD23	4:B:281:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:147:LEU:HB3	3:A:205:VAL:HG11	1.88	0.56
2:J:12:DA:H2"	2:J:13:DG:H5"	1.87	0.56
3:A:126:VAL:CG2	3:A:127:THR:N	2.69	0.56
4:B:310:ARG:O	4:B:312:LEU:HD12	2.04	0.56
3:A:50:LEU:HD12	3:A:50:LEU:O	2.04	0.56
4:B:295:LEU:HD23	4:B:299:SER:CB	2.34	0.56
3:A:151:ALA:HB2	3:A:205:VAL:HG21	1.88	0.56
3:A:42:ILE:CG1	3:A:70:ILE:HD11	2.35	0.56
4:B:253:LEU:HA	4:B:278:ILE:CG1	2.36	0.55
4:E:257:VAL:HG21	4:E:275:ILE:O	2.06	0.55
4:E:269:CYS:O	4:E:273:GLU:HB2	2.06	0.55
3:A:121:ALA:O	3:A:125:GLN:HG3	2.07	0.55
4:B:302:GLU:HG3	4:B:303:ILE:N	2.20	0.54
4:B:251:PRO:O	4:B:254:LEU:HG	2.07	0.54
4:B:253:LEU:HB3	4:B:321:TRP:HH2	1.72	0.54
1:K:27:DT:H1'	1:K:26:DC:H5'	1.89	0.54
3:A:183:VAL:O	3:A:187:LEU:HB2	2.08	0.54
4:E:306:VAL:O	4:E:310:ARG:HG2	2.07	0.53
1:K:31:DT:H6	1:K:31:DT:H5'	1.73	0.53
4:E:284:ARG:NH1	4:E:288:GLU:HB3	2.24	0.53
1:K:29:DT:H2"	1:K:28:DT:C5'	2.37	0.53
3:A:159:HIS:CE1	3:A:160:PRO:HG2	2.44	0.53
4:E:290:LEU:CD2	4:E:300:LEU:HD13	2.39	0.52
4:E:290:LEU:HD21	4:E:300:LEU:CD2	2.37	0.52
4:B:283:GLN:NE2	4:B:318:LEU:HD11	2.24	0.52
3:A:71:GLY:HA2	5:A:679:CMP:O3'	2.10	0.52
3:A:71:GLY:HA2	5:A:679:CMP:O2P	2.09	0.52
4:E:301:THR:HA	4:E:304:LYS:HE2	1.92	0.52
3:A:40:TYR:N	3:A:40:TYR:HD2	2.07	0.51
4:E:253:LEU:HA	4:E:278:ILE:CG1	2.39	0.51
3:A:38:THR:HG22	3:A:39:LEU:N	2.25	0.51
3:A:39:LEU:C	3:A:40:TYR:HD2	2.14	0.51
4:E:284:ARG:CB	4:E:284:ARG:HH11	2.24	0.51
3:A:40:TYR:CD2	3:A:40:TYR:N	2.78	0.51
3:A:137:LEU:HD12	3:A:137:LEU:N	2.26	0.51
4:B:299:SER:O	4:B:303:ILE:HG12	2.12	0.50
4:B:289:LEU:CD1	4:B:314:LEU:HD21	2.42	0.50
1:K:32:DT:H1'	1:K:31:DT:H5"	1.93	0.50
3:A:192:ASP:C	3:A:194:ASN:N	2.65	0.50
3:A:159:HIS:CG	3:A:160:PRO:HD2	2.47	0.50
4:E:281:LEU:O	4:E:284:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:250:ASP:HB3	4:B:253:LEU:HD13	1.94	0.50
1:K:25:DC:C2'	1:K:24:DT:H71	2.41	0.49
2:J:14:DA:H1'	2:J:15:DT:C5'	2.43	0.49
3:A:47:VAL:HG23	3:A:88:ALA:HA	1.94	0.49
4:B:309:SER:C	4:B:311:GLY:H	2.16	0.49
4:B:271:LYS:HE2	6:B:15:HOH:O	2.12	0.49
3:A:147:LEU:HB3	3:A:205:VAL:CG1	2.41	0.49
3:A:47:VAL:HA	3:A:89:LYS:H	1.77	0.49
2:J:14:DA:H1'	2:J:15:DT:H5"	1.95	0.49
3:A:196:ILE:HG22	3:A:205:VAL:HA	1.94	0.49
4:E:250:ASP:O	4:E:254:LEU:HD13	2.13	0.49
3:A:142:ARG:NH1	3:A:176:VAL:O	2.46	0.48
3:A:186:ILE:N	3:A:186:ILE:HD12	2.29	0.48
3:A:192:ASP:O	3:A:194:ASN:N	2.46	0.48
4:E:277:TYR:C	4:E:279:GLY:H	2.17	0.48
4:B:281:LEU:O	4:B:284:ARG:HB2	2.13	0.48
4:E:277:TYR:O	4:E:279:GLY:N	2.46	0.48
4:E:301:THR:HA	4:E:304:LYS:HE3	1.96	0.48
4:B:256:PRO:HA	4:B:277:TYR:HA	1.95	0.48
4:E:260:LEU:O	4:E:261:GLU:O	2.32	0.48
4:E:305:ASP:HA	4:E:308:ALA:HB2	1.96	0.47
4:E:255:ARG:HG3	4:E:259:ASP:HB3	1.95	0.47
2:J:12:DA:C2'	2:J:13:DG:H5"	2.44	0.47
1:K:31:DT:C6	1:K:31:DT:H5'	2.49	0.47
3:A:141:GLY:O	3:A:144:ALA:HB3	2.14	0.47
4:B:273:GLU:OE1	4:B:273:GLU:HA	2.15	0.47
4:B:283:GLN:O	4:B:283:GLN:HG3	2.14	0.47
3:A:169:ARG:NH2	3:A:200:GLY:O	2.48	0.47
4:E:277:TYR:C	4:E:279:GLY:N	2.68	0.47
4:E:257:VAL:HG23	4:E:258:ASP:H	1.78	0.47
4:E:305:ASP:O	4:E:308:ALA:HB3	2.15	0.47
3:A:122:ARG:NH1	6:A:684:HOH:O	2.48	0.47
3:A:186:ILE:O	3:A:190:LEU:HG	2.15	0.47
3:A:110:PRO:O	3:A:111:ASP:C	2.53	0.47
4:E:290:LEU:HD21	4:E:300:LEU:HD13	1.96	0.47
4:B:300:LEU:O	4:B:300:LEU:HD13	2.15	0.47
3:A:29:LEU:HD12	3:A:29:LEU:N	2.29	0.46
4:B:262:LEU:HD13	4:B:266:SER:CB	2.44	0.46
4:E:257:VAL:CG2	4:E:258:ASP:N	2.79	0.46
3:A:38:THR:HB	3:A:40:TYR:HE2	1.80	0.46
3:A:115:ARG:O	3:A:118:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:257:VAL:HG11	4:E:275:ILE:HG22	1.98	0.45
4:B:284:ARG:HH11	4:B:284:ARG:HA	1.81	0.45
3:A:13:TRP:CH2	3:A:109:ASN:HB3	2.50	0.45
1:K:24:DT:H2"	1:K:23:DA:N7	2.32	0.45
4:E:285:THR:N	4:E:288:GLU:HG3	2.21	0.45
4:B:273:GLU:O	4:B:274:ALA:HB3	2.16	0.45
3:A:112:ILE:CG2	3:A:113:LEU:N	2.78	0.45
4:B:283:GLN:HA	4:B:316:MET:N	2.31	0.45
3:A:167:ILE:N	3:A:201:LYS:HG2	2.32	0.45
3:A:137:LEU:CD1	3:A:137:LEU:N	2.80	0.45
3:A:208:THR:O	3:A:209:ARG:CB	2.64	0.45
3:A:163:MET:HG2	3:A:208:THR:HB	1.99	0.45
4:B:250:ASP:OD1	4:B:251:PRO:HD2	2.16	0.44
4:E:256:PRO:HG2	4:E:259:ASP:HB2	1.99	0.44
3:A:155:ASP:OD2	3:A:155:ASP:N	2.49	0.44
3:A:73:LEU:HD12	5:A:679:CMP:C3'	2.36	0.44
4:B:288:GLU:HA	4:B:288:GLU:OE1	2.17	0.44
3:A:112:ILE:HG22	3:A:113:LEU:N	2.31	0.44
3:A:161:ASP:O	3:A:206:TYR:HA	2.18	0.44
1:K:19:DT:OP2	3:A:170:GLN:HG3	2.17	0.44
3:A:125:GLN:O	3:A:128:SER:HB2	2.18	0.44
1:K:33:DC:H2"	1:K:32:DT:O5'	2.18	0.44
2:J:12:DA:H2"	2:J:13:DG:C5'	2.47	0.44
3:A:52:LYS:HG2	3:A:58:GLU:HG2	1.99	0.44
3:A:140:THR:HA	3:A:186:ILE:HG21	2.00	0.44
3:A:124:LEU:O	3:A:125:GLN:C	2.56	0.44
3:A:149:ASN:O	3:A:152:LYS:HB2	2.17	0.44
4:E:280:ASP:N	4:E:280:ASP:OD2	2.45	0.44
3:A:186:ILE:H	3:A:186:ILE:HD12	1.82	0.43
1:K:20:DA:C2'	3:A:170:GLN:HE21	2.28	0.43
4:B:270:LEU:HB3	4:B:275:ILE:HB	2.00	0.43
3:A:126:VAL:HG23	3:A:127:THR:H	1.80	0.43
2:J:20:DT:H2"	2:J:21:DT:OP2	2.19	0.43
4:B:253:LEU:HD12	4:B:253:LEU:N	2.26	0.43
4:B:275:ILE:HG21	4:B:281:LEU:HB2	1.99	0.43
4:B:282:VAL:CG1	4:B:283:GLN:N	2.81	0.43
4:E:251:PRO:HA	4:E:254:LEU:CD2	2.46	0.43
2:J:16:DC:H2"	2:J:17:DA:C8	2.54	0.43
3:A:32:GLN:HB2	3:A:84:ALA:C	2.38	0.43
3:A:171:GLU:O	3:A:172:ILE:C	2.57	0.43
4:B:277:TYR:C	4:B:279:GLY:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:281:LEU:HD21	4:B:307:LEU:HD11	2.00	0.43
4:B:299:SER:O	4:B:302:GLU:HB3	2.19	0.43
4:E:257:VAL:O	4:E:260:LEU:CB	2.63	0.43
3:A:167:ILE:HG23	3:A:167:ILE:O	2.17	0.43
3:A:163:MET:HG3	3:A:208:THR:HG21	2.01	0.43
4:E:287:VAL:O	4:E:291:LYS:HG2	2.18	0.43
4:E:264:VAL:O	4:E:267:ALA:HB3	2.19	0.43
3:A:42:ILE:HG12	3:A:70:ILE:HD11	1.99	0.43
3:A:197:SER:HB3	3:A:204:VAL:HB	2.00	0.43
4:B:280:ASP:O	4:B:281:LEU:C	2.57	0.42
4:B:286:GLU:HG2	4:B:314:LEU:HD23	2.01	0.42
3:A:166:LYS:HA	3:A:201:LYS:O	2.19	0.42
4:E:255:ARG:O	4:E:278:ILE:HG23	2.19	0.42
4:B:279:GLY:O	4:B:282:VAL:HG12	2.20	0.42
4:B:289:LEU:O	4:B:295:LEU:HD13	2.18	0.42
4:B:306:VAL:CG2	4:B:307:LEU:N	2.82	0.42
3:A:195:LEU:C	3:A:206:TYR:CD2	2.93	0.42
4:E:286:GLU:O	4:E:289:LEU:HD12	2.20	0.42
4:B:251:PRO:HA	4:B:254:LEU:HD11	2.02	0.42
4:B:266:SER:O	4:B:269:CYS:HB2	2.19	0.42
4:B:307:LEU:O	4:B:312:LEU:N	2.52	0.42
3:A:190:LEU:HB2	3:A:196:ILE:HD11	2.02	0.42
3:A:163:MET:CG	3:A:208:THR:HG21	2.49	0.42
3:A:208:THR:O	3:A:209:ARG:CG	2.68	0.42
4:E:278:ILE:HD12	4:E:278:ILE:C	2.40	0.41
4:E:284:ARG:HH12	4:E:288:GLU:HB3	1.84	0.41
3:A:126:VAL:CG2	3:A:127:THR:H	2.32	0.41
4:B:293:PRO:O	4:B:294:ASN:HB2	2.19	0.41
4:E:250:ASP:O	4:E:254:LEU:CD1	2.68	0.41
4:E:260:LEU:HD11	4:E:307:LEU:HD11	2.03	0.41
4:E:285:THR:N	4:E:288:GLU:CG	2.78	0.41
2:J:32:DA:OP2	4:E:264:VAL:HG21	2.20	0.41
4:B:257:VAL:HG22	4:B:276:HIS:O	2.21	0.41
4:B:310:ARG:O	4:B:312:LEU:CD1	2.68	0.41
3:A:13:TRP:CZ2	3:A:108:VAL:CG2	3.04	0.41
4:B:319:GLU:OE2	4:B:320:ASN:N	2.54	0.41
3:A:72:GLU:CD	5:A:679:CMP:HO2'	2.24	0.40
4:B:278:ILE:HD12	4:B:278:ILE:O	2.20	0.40
3:A:168:THR:HG22	3:A:201:LYS:HE2	2.04	0.40
3:A:87:ARG:CG	3:A:87:ARG:HH11	2.32	0.40
3:A:29:LEU:N	3:A:29:LEU:CD1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:279:GLY:O	4:E:280:ASP:C	2.60	0.40
4:E:250:ASP:OD1	4:E:251:PRO:HD2	2.21	0.40
3:A:46:SER:OG	3:A:90:THR:HG23	2.21	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
3	A	199/209 (95%)	178 (89%)	18 (9%)	3 (2%)	13 46
4	B	70/84 (83%)	48 (69%)	19 (27%)	3 (4%)	3 19
4	E	64/84 (76%)	39 (61%)	22 (34%)	3 (5%)	3 17
All	All	333/377 (88%)	265 (80%)	59 (18%)	9 (3%)	6 31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	261	GLU
3	A	193	GLN
4	B	268	ASN
3	A	153	GLN
3	A	155	ASP
4	E	282	VAL
4	B	282	VAL
4	E	278	ILE
4	B	264	VAL

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
3	A	173/180 (96%)	162 (94%)	11 (6%)	22 57
4	B	64/74 (86%)	55 (86%)	9 (14%)	4 18
4	E	58/74 (78%)	49 (84%)	9 (16%)	3 14
All	All	295/328 (90%)	266 (90%)	29 (10%)	10 36

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	11	LEU
3	A	40	TYR
3	A	54	GLU
3	A	59	MET
3	A	61	LEU
3	A	70	ILE
3	A	96	GLU
3	A	112	ILE
3	A	119	GLN
3	A	145	GLN
3	A	169	ARG
4	B	258	ASP
4	B	259	ASP
4	B	282	VAL
4	B	284	ARG
4	B	285	THR
4	B	290	LEU
4	B	295	LEU
4	B	300	LEU
4	B	302	GLU
4	E	254	LEU
4	E	260	LEU
4	E	278	ILE
4	E	280	ASP
4	E	284	ARG
4	E	289	LEU

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Mol	Chain	Res	Type
4	E	298	LYS
4	E	306	VAL
4	E	312	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	17	HIS
3	A	66	GLN
3	A	133	ASN
3	A	170	GLN
3	A	193	GLN
4	B	268	ASN
4	E	268	ASN
4	E	283	GLN
4	E	294	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

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	$\#\|Z\|>2$
5	CMP	A	679	-	19,25,25	1.18	3 (15%)	18,39,39	1.87	3 (16%)

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
5	CMP	A	679	-	-	0/0/31/31	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	679	CMP	O3'-C3'	-2.33	1.41	1.44
5	A	679	CMP	O5'-C5'	-2.10	1.43	1.46
5	A	679	CMP	P-O3'	2.31	1.62	1.58

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	679	CMP	O3'-C3'-C4'	-5.78	106.10	110.72
5	A	679	CMP	C2'-C1'-N9	-2.87	109.90	114.29
5	A	679	CMP	O2P-P-O1P	3.27	119.21	108.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	679	CMP	7	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	K	20/20 (100%)	-0.33	0	100	100	72, 85, 152, 156	0
2	J	24/24 (100%)	-0.60	0	100	100	75, 97, 125, 143	0
3	A	201/209 (96%)	-0.51	0	100	100	52, 82, 128, 153	0
4	B	72/84 (85%)	-0.42	0	100	100	86, 126, 164, 180	0
4	E	66/84 (78%)	-0.37	0	100	100	90, 144, 176, 180	0
All	All	383/421 (90%)	-0.46	0	100	100	52, 99, 160, 180	0

There are no RSRZ outliers to report.

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 carbohydrates in this entry.

6.4 Ligands

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
5	CMP	A	679	22/22	0.97	0.15	-0.50	34,43,48,50	0

6.5 Other polymers (i)

There are no such residues in this entry.