WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 06:25 AM EDT

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PDB ID	:	3D1E
Title	:	Crystal structure of E. coli sliding clamp (beta) bound to a polymerase II peptide
Authors	:	Georgescu, R.E.; Yurieva, O.; Seung-Sup, K.; Kuriyan, J.; Kong, X.-P.; O'Donnell, M.
Deposited on	:	2008-05-05
Resolution	:	1.90 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
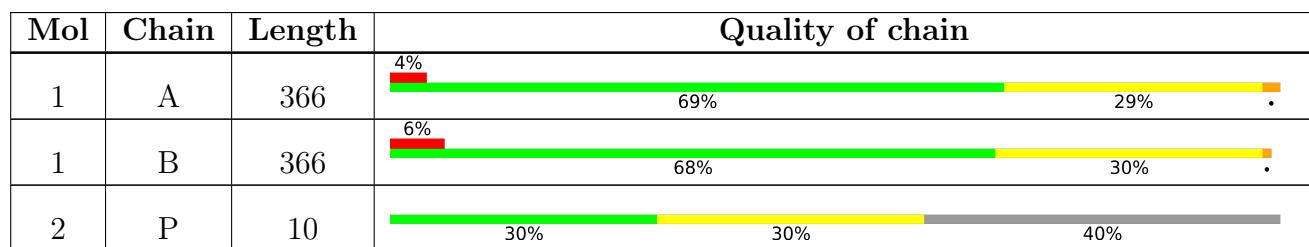
The reported resolution of this entry is 1.90 Å.

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	Percentile Ranks	Value
Clashscore		20
Ramachandran outliers		0.5%
Sidechain outliers		2.2%
RSRZ outliers		5.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	366	4% 69% 29% •
1	B	366	6% 68% 30% •
2	P	10	30% 30% 40%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6205 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 DNA polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			
1	B	366	Total	C	N	O	S	0	0	0
			2844	1786	498	541	19			

- Molecule 2 is a protein called decamer from polymerase II C-terminal.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			45	30	7	8			
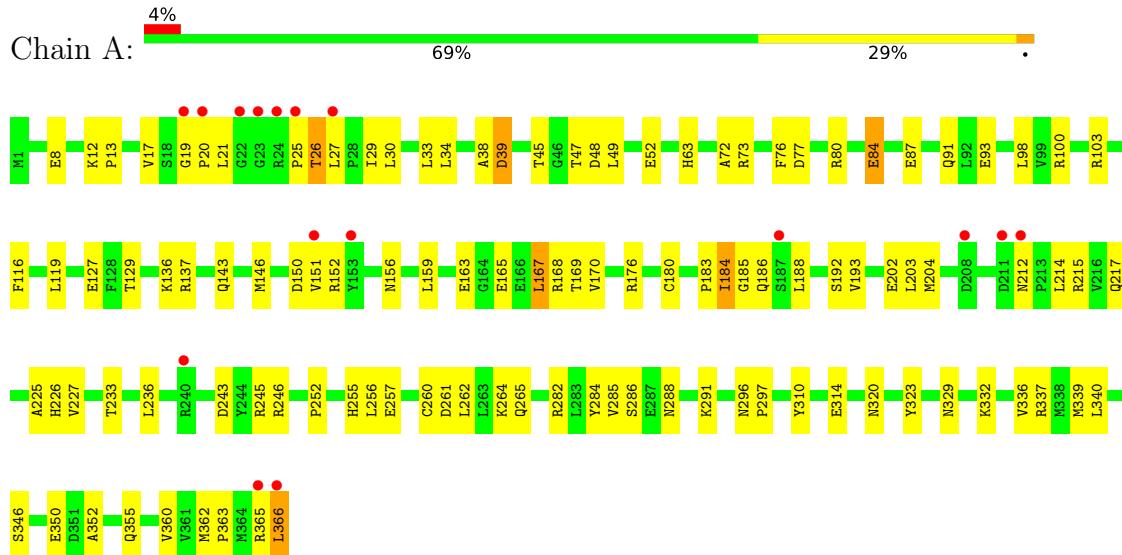
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total	O	0	0
			213	213		
3	B	253	Total	O	0	0
			253	253		
3	P	6	Total	O	0	0
			6	6		
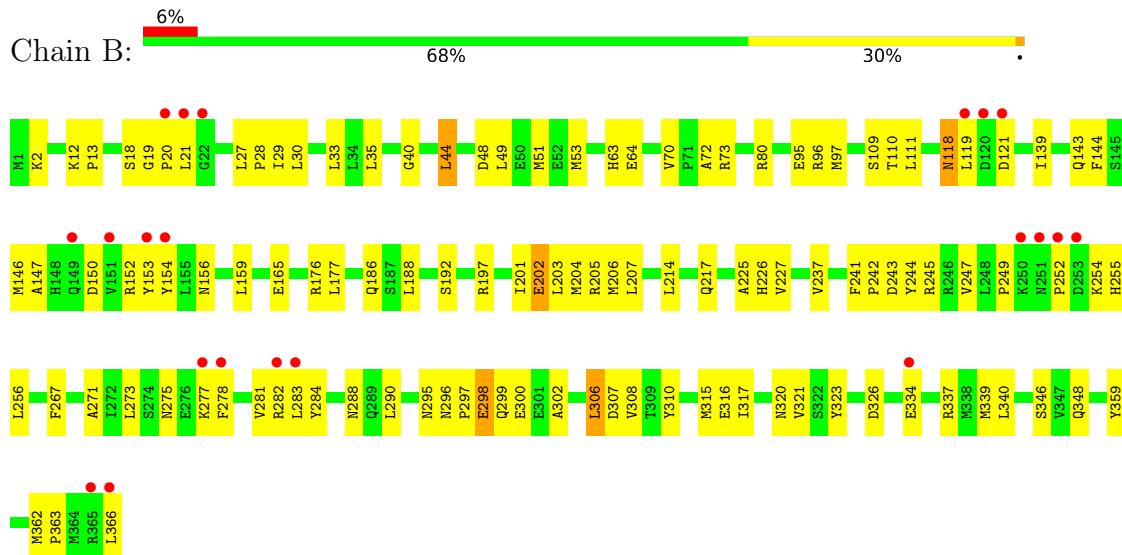
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
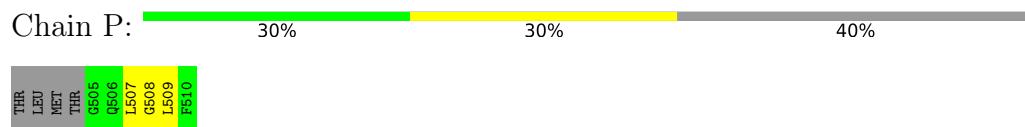
• Molecule 1: DNA polymerase III subunit beta

Chain A:

• Molecule 1: DNA polymerase III subunit beta

Chain B:

• Molecule 2: decamer from polymerase II C-terminal

Chain P:

30%　　　　30%　　　　40%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.14Å 69.87Å 73.12Å 112.89° 91.08° 99.28°	Depositor
Resolution (Å)	33.55 – 1.90 33.54 – 1.79	Depositor EDS
% Data completeness (in resolution range)	92.9 (33.55-1.90) 88.9 (33.54-1.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 1.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.261 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6205	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/2893	0.59	0/3915
1	B	0.33	0/2893	0.61	0/3915
2	P	0.54	0/45	0.53	0/57
All	All	0.33	0/5831	0.60	0/7887

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 (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	2844	0	2861	116	0
1	B	2844	0	2861	112	0
2	P	45	0	44	7	0
3	A	213	0	0	12	0
3	B	253	0	0	5	0
3	P	6	0	0	0	0
All	All	6205	0	5766	227	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 20.

All (227) 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:A:252:PRO:HB2	1:A:339:MET:HB3	1.53	0.91
1:B:177:LEU:HD13	1:B:247:VAL:HG11	1.52	0.90
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.54	0.87
1:B:197:ARG:HH11	1:B:197:ARG:HB3	1.37	0.87
1:B:346:SER:HA	1:B:363:PRO:HD3	1.58	0.86
1:A:365:ARG:NE	2:P:507:LEU:HD21	1.92	0.83
1:A:127:GLU:HG2	1:A:217:GLN:HG2	1.57	0.83
1:B:275:ASN:HD22	1:B:277:LYS:H	1.25	0.82
1:A:264:LYS:NZ	1:A:329:ASN:HD21	1.78	0.82
1:B:35:LEU:HD22	1:B:44:LEU:HD12	1.62	0.81
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.47	0.79
1:A:129:THR:HG23	1:A:215:ARG:HH11	1.50	0.75
1:A:184:ILE:HD13	1:A:184:ILE:H	1.51	0.75
1:B:27:LEU:HD23	1:B:28:PRO:HD2	1.71	0.73
1:B:159:LEU:HD11	1:B:192:SER:HB2	1.71	0.73
1:A:26:THR:HB	1:A:30:LEU:HD12	1.68	0.73
1:B:197:ARG:HB3	1:B:197:ARG:NH1	2.04	0.73
1:A:214:LEU:HD13	1:A:227:VAL:HG22	1.69	0.72
1:A:362:MET:HG2	2:P:509:LEU:HD23	1.72	0.72
1:B:282:ARG:HG2	1:B:284:TYR:CE1	2.25	0.72
1:A:119:LEU:HD12	1:A:233:THR:HG23	1.72	0.72
1:A:288:ASN:HD22	1:A:310:TYR:H	1.37	0.71
1:A:365:ARG:HE	2:P:507:LEU:HD21	1.54	0.71
1:B:249:PRO:HD2	1:B:348:GLN:HE21	1.56	0.71
1:A:193:VAL:HB	1:A:236:LEU:HD13	1.71	0.70
1:B:275:ASN:ND2	1:B:277:LYS:H	1.89	0.70
1:B:201:ILE:O	1:B:205:ARG:HG2	1.91	0.69
1:A:77:ASP:HA	1:A:80:ARG:HH12	1.56	0.69
1:B:275:ASN:HD21	1:B:277:LYS:HB2	1.56	0.69
1:B:366:LEU:HD12	1:B:366:LEU:OXT	1.92	0.68
1:B:12:LYS:HB3	1:B:13:PRO:HD3	1.76	0.68
1:B:339:MET:HE1	1:B:348:GLN:HG2	1.76	0.68
1:A:129:THR:HG22	1:A:215:ARG:HD3	1.75	0.68
1:A:27:LEU:HG	3:A:415:HOH:O	1.94	0.67
1:B:288:ASN:HD22	1:B:310:TYR:H	1.41	0.67
1:A:337:ARG:HH12	1:A:352:ALA:HA	1.60	0.65
1:B:275:ASN:ND2	1:B:277:LYS:HB2	2.12	0.65
1:B:35:LEU:HD22	1:B:44:LEU:CD1	2.27	0.65
1:A:362:MET:HG2	2:P:509:LEU:CD2	2.28	0.64
1:A:26:THR:HG22	1:A:27:LEU:H	1.64	0.63
1:B:186:GLN:HB2	1:B:188:LEU:HD11	1.78	0.63
1:A:26:THR:HG22	1:A:27:LEU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:O	1:B:49:LEU:HB2	1.99	0.62
1:B:255:HIS:CD2	1:B:337:ARG:HD3	2.34	0.62
1:A:337:ARG:NH1	1:A:352:ALA:HA	2.14	0.62
1:A:137:ARG:NH1	1:A:180:CYS:SG	2.73	0.61
1:B:267:PHE:CE1	1:B:283:LEU:HD21	2.35	0.61
1:A:52:GLU:HB3	1:A:233:THR:HG22	1.81	0.61
1:B:267:PHE:CZ	1:B:283:LEU:HD21	2.34	0.61
1:A:77:ASP:HA	1:A:80:ARG:NH1	2.16	0.61
1:B:339:MET:CE	1:B:348:GLN:HG2	2.31	0.60
1:A:332:LYS:HD3	3:A:550:HOH:O	2.02	0.60
1:B:144:PHE:CD2	1:B:326:ASP:HB3	2.36	0.60
1:A:98:LEU:HD21	1:A:100:ARG:HD3	1.84	0.59
1:B:296:ASN:HB2	1:B:297:PRO:CD	2.33	0.59
1:A:262:LEU:HD23	3:A:487:HOH:O	2.03	0.58
1:B:27:LEU:HD23	1:B:28:PRO:CD	2.34	0.58
1:A:119:LEU:HD12	1:A:233:THR:CG2	2.34	0.57
1:B:288:ASN:ND2	1:B:310:TYR:H	2.00	0.57
1:A:184:ILE:HD13	1:A:184:ILE:N	2.20	0.57
1:A:346:SER:HB3	1:A:362:MET:SD	2.44	0.57
1:B:290:LEU:HB3	1:B:306:LEU:CD1	2.34	0.57
1:A:129:THR:CG2	1:A:215:ARG:HH11	2.17	0.57
1:B:203:LEU:O	1:B:206:MET:HG2	2.03	0.57
1:A:260:CYS:HB2	1:A:336:VAL:HG13	1.87	0.56
1:B:147:ALA:HB3	1:B:156:ASN:HD22	1.70	0.56
1:B:275:ASN:ND2	1:B:278:PHE:H	2.03	0.56
1:A:12:LYS:HB3	1:A:13:PRO:HD3	1.87	0.56
1:A:137:ARG:HH11	1:A:137:ARG:CG	2.16	0.56
1:A:264:LYS:HZ3	1:A:329:ASN:HD21	1.51	0.56
1:B:96:ARG:HG2	1:B:96:ARG:HH11	1.71	0.56
1:B:346:SER:HB3	1:B:362:MET:SD	2.46	0.56
1:A:150:ASP:H	1:A:156:ASN:HD21	1.52	0.56
1:B:275:ASN:HD22	1:B:277:LYS:N	2.00	0.56
1:A:346:SER:HA	1:A:363:PRO:HD3	1.88	0.56
1:B:165:GLU:HA	1:B:186:GLN:O	2.07	0.55
1:B:244:TYR:O	1:B:247:VAL:HG12	2.07	0.54
1:A:48:ASP:O	1:A:49:LEU:HB2	2.08	0.54
1:B:118:ASN:O	1:B:119:LEU:HB2	2.07	0.54
1:A:163:GLU:CD	1:A:168:ARG:HH22	2.10	0.54
1:A:20:PRO:HD3	1:A:202:GLU:OE2	2.08	0.54
1:A:167:LEU:HD23	1:A:168:ARG:N	2.22	0.54
1:B:27:LEU:CD2	3:B:550:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLU:HG2	1:B:96:ARG:HG2	1.91	0.53
1:A:340:LEU:N	1:A:340:LEU:HD12	2.23	0.53
1:B:35:LEU:CD2	1:B:44:LEU:HD12	2.36	0.53
1:B:271:ALA:HB2	1:B:321:VAL:HG21	1.90	0.53
1:A:129:THR:HG23	1:A:215:ARG:NH1	2.21	0.53
1:B:243:ASP:OD1	1:B:245:ARG:HG3	2.09	0.52
1:B:73:ARG:NH2	1:B:80:ARG:HH21	2.07	0.52
1:B:290:LEU:HB3	1:B:306:LEU:HD11	1.92	0.52
1:B:275:ASN:HD22	1:B:278:PHE:H	1.55	0.52
1:A:217:GLN:OE1	1:A:226:HIS:HE1	1.92	0.52
1:B:96:ARG:HG2	1:B:96:ARG:NH1	2.25	0.52
1:A:129:THR:H	1:A:186:GLN:HE22	1.57	0.52
1:A:282:ARG:NH2	1:A:366:LEU:HD23	2.25	0.52
1:B:244:TYR:HA	1:B:247:VAL:HG12	1.92	0.52
1:B:298:GLU:OE1	1:B:298:GLU:N	2.43	0.52
1:A:33:LEU:HG	1:A:72:ALA:HB2	1.92	0.51
1:A:91:GLN:NE2	1:A:93:GLU:OE2	2.41	0.51
1:A:186:GLN:O	1:A:188:LEU:HG	2.09	0.51
1:B:317:ILE:HD11	1:B:363:PRO:HB3	1.92	0.51
1:A:136:LYS:HG3	1:A:204:MET:CE	2.41	0.51
1:A:337:ARG:NH1	1:A:337:ARG:HB2	2.26	0.51
1:B:284:TYR:CD2	1:B:316:GLU:HG2	2.46	0.51
1:A:150:ASP:OD1	1:A:152:ARG:HD3	2.12	0.50
1:A:284:TYR:HB2	1:A:291:LYS:HB3	1.92	0.50
1:B:156:ASN:O	1:B:197:ARG:HB2	2.10	0.50
1:A:288:ASN:ND2	1:A:310:TYR:H	2.07	0.50
1:B:18:SER:HA	1:B:21:LEU:HD13	1.93	0.50
1:B:27:LEU:HB3	1:B:30:LEU:HG	1.93	0.50
1:B:217:GLN:NE2	1:B:226:HIS:NE2	2.59	0.50
1:A:52:GLU:HB3	1:A:233:THR:CG2	2.41	0.50
1:A:246:ARG:NH2	3:A:545:HOH:O	2.42	0.49
1:A:255:HIS:CD2	1:A:339:MET:HG2	2.47	0.49
1:B:150:ASP:H	1:B:156:ASN:HD21	1.60	0.49
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.93	0.49
1:B:21:LEU:N	1:B:21:LEU:HD12	2.28	0.49
1:A:214:LEU:HD13	1:A:227:VAL:CG2	2.39	0.49
1:A:119:LEU:CD1	1:A:233:THR:HG23	2.42	0.49
1:B:20:PRO:HD3	3:B:494:HOH:O	2.13	0.48
1:A:257:GLU:HB2	3:A:576:HOH:O	2.12	0.48
1:A:151:VAL:HG23	1:A:152:ARG:N	2.28	0.48
1:B:296:ASN:HB2	1:B:297:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:LEU:C	1:B:256:LEU:HD23	2.33	0.48
1:A:136:LYS:HG3	1:A:204:MET:HE1	1.96	0.48
1:B:282:ARG:NH2	1:B:366:LEU:HB3	2.29	0.48
1:B:245:ARG:NH1	3:B:669:HOH:O	2.47	0.48
1:A:26:THR:CG2	1:A:27:LEU:H	2.22	0.47
1:B:20:PRO:HG2	1:B:21:LEU:HD12	1.96	0.47
1:B:139:ILE:HG21	1:B:204:MET:HG2	1.96	0.47
1:A:8:GLU:OE1	1:A:84:GLU:HG2	2.15	0.47
1:A:168:ARG:HG3	1:A:180:CYS:O	2.15	0.47
1:A:363:PRO:HG2	2:P:507:LEU:HD12	1.96	0.47
1:B:214:LEU:HD13	1:B:227:VAL:CG2	2.45	0.47
1:A:137:ARG:HG3	1:A:137:ARG:NH1	2.25	0.47
1:A:27:LEU:HD23	1:A:29:ILE:CG2	2.45	0.46
1:B:298:GLU:O	1:B:299:GLN:HB2	2.15	0.46
1:A:284:TYR:HB3	3:A:566:HOH:O	2.16	0.46
1:A:33:LEU:HG	1:A:72:ALA:CB	2.46	0.46
1:A:127:GLU:CG	1:A:217:GLN:HG2	2.38	0.46
1:A:264:LYS:HZ1	1:A:329:ASN:HD21	1.56	0.46
1:A:19:GLY:N	1:A:20:PRO:HD2	2.31	0.46
1:B:154:TYR:HA	1:B:237:VAL:HG11	1.97	0.46
1:A:159:LEU:O	1:A:169:THR:HA	2.15	0.46
1:A:296:ASN:HB2	1:A:297:PRO:CD	2.46	0.46
1:B:297:PRO:HB2	1:B:298:GLU:OE1	2.15	0.46
1:B:252:PRO:CG	1:B:339:MET:HB3	2.46	0.45
1:A:17:VAL:O	1:A:20:PRO:HD2	2.16	0.45
1:B:118:ASN:H	1:B:118:ASN:HD22	1.65	0.45
1:B:282:ARG:HH21	1:B:366:LEU:HB3	1.80	0.45
1:B:40:GLY:HA2	1:B:63:HIS:NE2	2.32	0.45
1:B:340:LEU:HD12	1:B:340:LEU:N	2.32	0.45
1:A:261:ASP:O	1:A:265:GLN:HG2	2.16	0.45
1:B:95:GLU:HG2	1:B:96:ARG:CG	2.47	0.45
1:A:129:THR:HG22	1:A:215:ARG:CD	2.45	0.44
1:A:350:GLU:OE2	1:A:355:GLN:HG2	2.18	0.44
1:B:2:LYS:NZ	1:B:64:GLU:CD	2.70	0.44
1:A:73:ARG:HH21	1:A:76:PHE:HD2	1.64	0.44
1:A:8:GLU:OE2	1:A:8:GLU:N	2.50	0.44
1:B:282:ARG:HH12	1:B:316:GLU:C	2.20	0.44
1:B:334:GLU:N	1:B:334:GLU:OE2	2.51	0.44
1:A:27:LEU:HD23	1:A:29:ILE:HG22	1.99	0.44
1:A:137:ARG:NH1	1:A:137:ARG:CG	2.76	0.44
1:A:143:GLN:HG3	1:A:146:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:NH2	1:B:109:SER:OG	2.50	0.44
1:A:360:VAL:HG12	2:P:509:LEU:HD21	2.00	0.44
1:B:27:LEU:HD22	1:B:29:ILE:HG22	2.00	0.44
1:A:212:ASN:HB3	3:A:564:HOH:O	2.17	0.44
1:B:139:ILE:HG21	1:B:204:MET:CG	2.48	0.44
1:A:226:HIS:HB3	3:A:462:HOH:O	2.16	0.43
1:A:362:MET:HG3	2:P:508:GLY:C	2.38	0.43
1:B:241:PHE:CG	1:B:242:PRO:HD2	2.53	0.43
1:B:295:ASN:HA	1:B:300:GLU:O	2.17	0.43
1:A:87:GLU:HG2	3:A:507:HOH:O	2.19	0.43
1:B:70:VAL:HG11	1:B:97:MET:SD	2.58	0.43
1:B:177:LEU:HD23	1:B:177:LEU:C	2.39	0.43
1:B:290:LEU:HB3	1:B:306:LEU:HD12	1.99	0.43
1:B:152:ARG:O	1:B:154:TYR:N	2.52	0.43
1:B:249:PRO:HD2	1:B:348:GLN:NE2	2.30	0.43
1:B:282:ARG:HH12	1:B:317:ILE:N	2.16	0.43
1:A:256:LEU:C	1:A:256:LEU:HD23	2.39	0.43
1:A:285:VAL:HG22	1:A:310:TYR:CD2	2.54	0.43
1:A:100:ARG:HG3	1:A:100:ARG:HH11	1.83	0.43
1:A:243:ASP:OD1	1:A:245:ARG:HG3	2.19	0.43
1:B:44:LEU:HD22	1:B:44:LEU:N	2.34	0.43
1:B:53:MET:HB2	3:B:494:HOH:O	2.18	0.43
1:B:118:ASN:HD22	1:B:118:ASN:N	2.16	0.43
1:A:38:ALA:O	1:A:39:ASP:HB2	2.18	0.42
1:B:254:LYS:HD2	1:B:315:MET:CE	2.49	0.42
1:A:159:LEU:HD11	1:A:192:SER:HB3	2.01	0.42
1:B:306:LEU:HD13	1:B:308:VAL:CG1	2.50	0.42
1:A:264:LYS:NZ	3:A:539:HOH:O	2.51	0.42
1:A:103:ARG:HH22	1:B:307:ASP:CG	2.23	0.42
1:A:184:ILE:HD11	1:A:188:LEU:HD11	2.01	0.42
1:A:320:ASN:HB3	1:A:323:TYR:CD2	2.55	0.42
1:B:298:GLU:CD	1:B:298:GLU:H	2.23	0.42
1:B:348:GLN:HA	1:B:359:TYR:O	2.19	0.42
1:A:47:THR:HG22	1:A:116:PHE:CZ	2.55	0.42
1:A:80:ARG:NH1	1:A:80:ARG:HB3	2.35	0.42
1:A:286:SER:HA	1:A:314:GLU:HG2	2.02	0.42
1:A:365:ARG:O	1:A:366:LEU:HB2	2.20	0.41
1:B:275:ASN:HA	3:B:624:HOH:O	2.21	0.41
1:B:281:VAL:CG1	1:B:321:VAL:HB	2.50	0.41
1:B:51:MET:CE	1:B:202:GLU:HG3	2.50	0.41
1:A:26:THR:HB	1:A:30:LEU:CD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASN:HB2	1:A:297:PRO:HD2	2.03	0.41
1:A:337:ARG:NH1	1:A:337:ARG:CB	2.83	0.41
1:B:19:GLY:N	1:B:20:PRO:HD2	2.35	0.41
1:B:143:GLN:HG3	1:B:146:MET:HE2	2.02	0.41
1:B:320:ASN:HB3	1:B:323:TYR:CD2	2.56	0.41
1:A:159:LEU:HB3	1:A:170:VAL:HB	2.03	0.41
1:A:21:LEU:HA	3:A:528:HOH:O	2.20	0.41
1:B:70:VAL:HG12	1:B:110:THR:HG22	2.03	0.41
1:B:73:ARG:HH22	1:B:80:ARG:HH21	1.68	0.41
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.95	0.41
1:B:197:ARG:HH11	1:B:197:ARG:CB	2.20	0.41
1:B:273:LEU:HD12	1:B:302:ALA:HB2	2.03	0.41
1:A:34:LEU:HB3	1:A:45:THR:HB	2.03	0.40
1:A:63:HIS:HB3	3:A:426:HOH:O	2.20	0.40
1:A:165:GLU:O	1:A:183:PRO:HA	2.22	0.40
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.36	0.40
1:A:282:ARG:HH21	1:A:366:LEU:HD23	1.87	0.40
1:B:275:ASN:ND2	1:B:277:LYS:N	2.64	0.40
1:A:165:GLU:CD	1:A:185:GLY:HA2	2.42	0.40
1:B:297:PRO:C	1:B:299:GLN:H	2.24	0.40
1:B:33:LEU:HG	1:B:72:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	364/366 (100%)	347 (95%)	15 (4%)	2 (0%)	29	18
1	B	364/366 (100%)	347 (95%)	15 (4%)	2 (0%)	29	18
2	P	4/10 (40%)	4 (100%)	0	0	100	100
All	All	732/742 (99%)	698 (95%)	30 (4%)	4 (0%)	29	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	B	121	ASP
1	B	153	TYR
1	A	25	PRO

5.3.2 Protein sidechains ⓘ

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	313/313 (100%)	306 (98%)	7 (2%)	52	47
1	B	313/313 (100%)	306 (98%)	7 (2%)	52	47
2	P	4/8 (50%)	4 (100%)	0	100	100
All	All	630/634 (99%)	616 (98%)	14 (2%)	52	47

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

Mol	Chain	Res	Type
1	A	39	ASP
1	A	84	GLU
1	A	167	LEU
1	A	176	ARG
1	A	184	ILE
1	A	203	LEU
1	A	366	LEU
1	B	44	LEU
1	B	118	ASN
1	B	176	ARG
1	B	202	GLU
1	B	207	LEU
1	B	298	GLU
1	B	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	32	ASN
1	A	36	GLN
1	A	123	GLN
1	A	143	GLN
1	A	149	GLN
1	A	156	ASN
1	A	186	GLN
1	A	221	ASN
1	A	226	HIS
1	A	288	ASN
1	A	295	ASN
1	A	329	ASN
1	A	355	GLN
1	B	16	GLN
1	B	118	ASN
1	B	123	GLN
1	B	143	GLN
1	B	149	GLN
1	B	156	ASN
1	B	191	HIS
1	B	217	GLN
1	B	255	HIS
1	B	275	ASN
1	B	288	ASN
1	B	329	ASN
1	B	348	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	366/366 (100%)	0.20	16 (4%)	34	37	18, 34, 56, 84	0
1	B	366/366 (100%)	0.11	21 (5%)	23	26	15, 29, 52, 66	0
2	P	6/10 (60%)	0.88	0	100	100	39, 45, 49, 52	0
All	All	738/742 (99%)	0.16	37 (5%)	28	32	15, 33, 54, 84	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	GLY	7.4
1	A	24	ARG	7.4
1	B	120	ASP	6.1
1	A	366	LEU	5.8
1	B	366	LEU	5.5
1	B	153	TYR	4.6
1	A	208	ASP	4.5
1	A	22	GLY	4.1
1	A	27	LEU	3.9
1	B	22	GLY	3.8
1	B	251	ASN	3.8
1	A	25	PRO	3.8
1	A	365	ARG	3.4
1	A	20	PRO	3.3
1	B	252	PRO	3.2
1	B	365	ARG	3.0
1	B	20	PRO	3.0
1	B	250	LYS	3.0
1	B	278	PHE	2.9
1	A	19	GLY	2.7
1	A	187	SER	2.7
1	B	21	LEU	2.6
1	B	149	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	253	ASP	2.4
1	B	282	ARG	2.3
1	A	211	ASP	2.3
1	A	240	ARG	2.3
1	B	151	VAL	2.3
1	B	277	LYS	2.2
1	B	119	LEU	2.2
1	B	334	GLU	2.1
1	B	121	ASP	2.1
1	A	212	ASN	2.1
1	B	154	TYR	2.1
1	A	151	VAL	2.1
1	B	283	LEU	2.0
1	A	153	TYR	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 monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.