



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 07:51 AM EST

PDB ID : 1JQL  
Title : Mechanism of Processivity Clamp Opening by the Delta Subunit Wrench of the Clamp Loader Complex of E. coli DNA Polymerase III: Structure of beta-delta (1-140)  
Authors : Jeruzalmi, D.; Yurieva, O.; Zhao, Y.; Young, M.; Stewart, J.; Hingorani, M.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2001-08-07  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

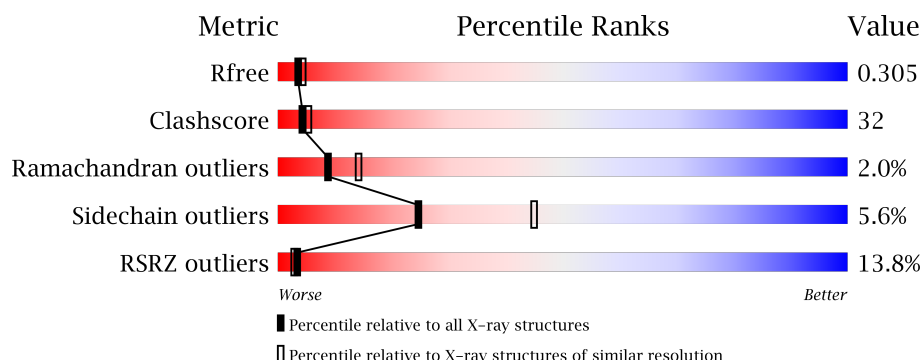
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	366	<div> <div>5%</div> <div>63%</div> <div>33%</div> <div>.</div> </div>
2	B	140	<div> <div>36%</div> <div>30%</div> <div>64%</div> <div>6%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3932 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, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2837	1780	498	540	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	ILE	ENGINEERED	UNP P0A988
A	273	ALA	LEU	ENGINEERED	UNP P0A988

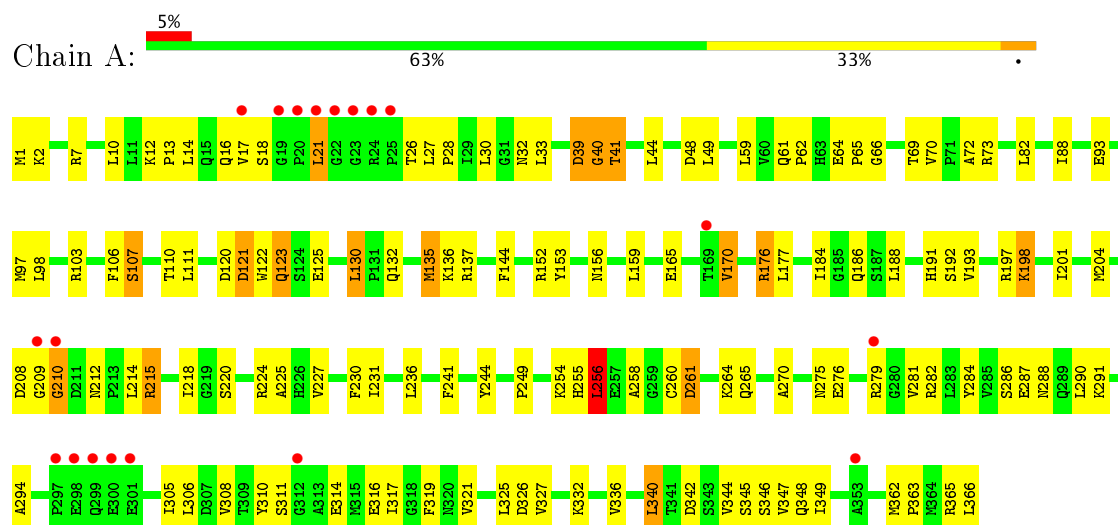
- Molecule 2 is a protein called DNA Polymerase III, DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	140	Total	C	N	O	S	0	0	0
			1095	691	193	207	4			

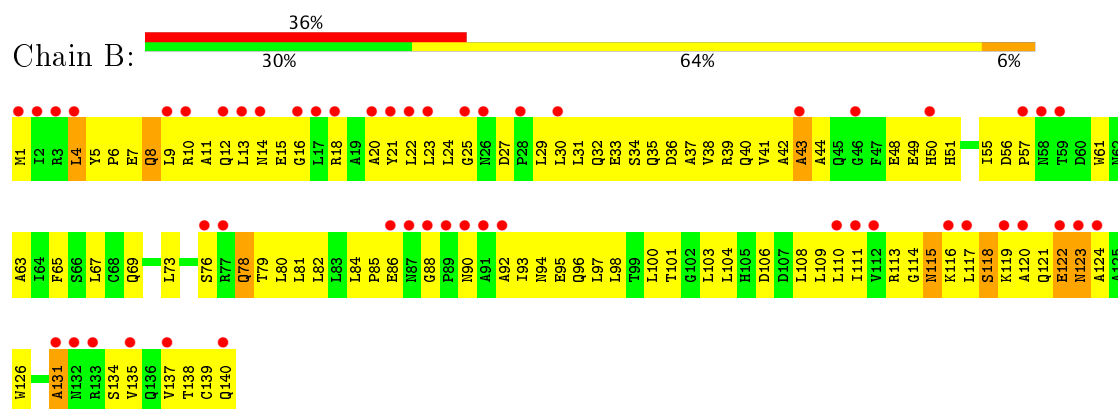
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, BETA CHAIN



#### • Molecule 2: DNA Polymerase III, DELTA SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.10Å 110.10Å 134.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	500.00 – 2.50 19.88 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.7 (500.00-2.50) 93.2 (19.88-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.249 , 0.294 0.266 , 0.305	Depositor DCC
$R_{free}$ test set	2627 reflections (8.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3932	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/2886	0.77	2/3907 (0.1%)
2	B	0.36	0/1113	0.73	1/1513 (0.1%)
All	All	0.45	0/3999	0.76	3/5420 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	256	LEU	CA-CB-CG	5.69	128.39	115.30
2	B	103	LEU	CA-CB-CG	5.20	127.26	115.30

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	2837	0	2849	119	0
2	B	1095	0	1098	139	0
All	All	3932	0	3947	253	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 32.

All (253) 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:184:ILE:HD11	1:A:188:LEU:HD11	1.25	1.11
2:B:4:LEU:HD22	2:B:12:GLN:HG3	1.27	1.09
2:B:48:GLU:HG2	2:B:76:SER:HB2	1.34	1.05
1:A:152:ARG:HD3	2:B:48:GLU:HG3	1.41	1.00
1:A:32:ASN:HD22	1:A:69:THR:HG22	1.32	0.92
1:A:32:ASN:HB3	1:A:69:THR:HG23	1.53	0.89
2:B:4:LEU:HD22	2:B:12:GLN:CG	2.08	0.84
1:A:215:ARG:HH11	1:A:215:ARG:HG2	1.42	0.82
1:A:93:GLU:OE1	1:A:98:LEU:HD11	1.79	0.82
2:B:7:GLU:HG3	2:B:8:GLN:HG3	1.62	0.82
2:B:6:PRO:HG2	2:B:30:LEU:HD13	1.62	0.81
2:B:56:ASP:HB2	2:B:57:PRO:HD2	1.60	0.81
1:A:135:MET:HG3	1:A:214:LEU:HD23	1.63	0.80
2:B:20:ALA:HB3	2:B:134:SER:HB3	1.63	0.79
1:A:32:ASN:HD22	1:A:69:THR:CG2	1.96	0.79
1:A:135:MET:HG3	1:A:214:LEU:CD2	2.13	0.78
1:A:340:LEU:HD23	1:A:347:VAL:HG22	1.66	0.78
2:B:4:LEU:HD23	2:B:8:GLN:HB2	1.66	0.77
2:B:97:LEU:O	2:B:101:THR:HG23	1.83	0.77
2:B:1:MET:HB2	2:B:131:ALA:O	1.85	0.77
2:B:118:SER:HB2	2:B:121:GLN:HB2	1.66	0.77
2:B:39:ARG:NH2	2:B:50:HIS:HB3	2.01	0.76
1:A:215:ARG:HG2	1:A:215:ARG:NH1	1.99	0.75
1:A:12:LYS:HB2	1:A:13:PRO:HD3	1.69	0.74
2:B:48:GLU:HG2	2:B:76:SER:CB	2.17	0.73
2:B:81:LEU:C	2:B:82:LEU:HD12	2.08	0.73
1:A:69:THR:HB	1:A:111:LEU:O	1.89	0.73
1:A:258:ALA:HB2	1:A:308:VAL:HG23	1.72	0.72
1:A:1:MET:HB3	1:A:66:GLY:HA3	1.71	0.72
2:B:6:PRO:HD3	2:B:138:THR:O	1.88	0.71
2:B:118:SER:HB3	2:B:121:GLN:HG3	1.72	0.71
2:B:113:ARG:HG2	2:B:114:GLY:H	1.55	0.70
2:B:113:ARG:HG2	2:B:114:GLY:N	2.04	0.70
1:A:317:ILE:HD11	1:A:363:PRO:HB3	1.73	0.70
2:B:4:LEU:CD2	2:B:12:GLN:HG3	2.14	0.69
2:B:41:VAL:O	2:B:44:ALA:HB3	1.93	0.68
2:B:80:LEU:HG	2:B:82:LEU:HD11	1.74	0.68
1:A:136:LYS:HG3	1:A:204:MET:CE	2.24	0.68
1:A:214:LEU:HD13	1:A:227:VAL:HG22	1.75	0.68
1:A:365:ARG:HG2	2:B:69:GLN:O	1.93	0.68
1:A:165:GLU:HA	1:A:186:GLN:O	1.94	0.67
1:A:184:ILE:HD11	1:A:188:LEU:CD1	2.16	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ILE:HD12	1:A:218:ILE:N	2.09	0.67
1:A:319:PHE:HZ	1:A:347:VAL:HG21	1.60	0.66
1:A:290:LEU:HD23	1:A:306:LEU:HD12	1.76	0.66
2:B:36:ASP:O	2:B:40:GLN:HB2	1.95	0.66
1:A:340:LEU:HD23	1:A:347:VAL:CG2	2.26	0.65
2:B:86:GLU:HA	2:B:115:ASN:HD21	1.61	0.65
2:B:117:LEU:HD13	2:B:122:GLU:HG2	1.79	0.65
1:A:362:MET:HG2	2:B:73:LEU:HD23	1.79	0.64
1:A:61:GLN:HB3	1:A:62:PRO:HD2	1.79	0.64
2:B:117:LEU:HD22	2:B:122:GLU:HG2	1.79	0.64
1:A:44:LEU:HD12	1:A:44:LEU:N	2.13	0.64
2:B:37:ALA:O	2:B:41:VAL:HG23	1.98	0.64
2:B:63:ALA:O	2:B:67:LEU:HB2	1.98	0.64
2:B:13:LEU:HG	2:B:41:VAL:HG21	1.80	0.64
2:B:4:LEU:CD2	2:B:8:GLN:HB2	2.28	0.64
2:B:15:GLU:HG3	2:B:16:GLY:N	2.13	0.63
2:B:22:LEU:N	2:B:22:LEU:HD22	2.13	0.63
1:A:214:LEU:HD12	1:A:215:ARG:H	1.64	0.63
1:A:33:LEU:HG	1:A:72:ALA:HB2	1.79	0.63
2:B:118:SER:CB	2:B:121:GLN:HG3	2.27	0.63
2:B:25:GLY:O	2:B:31:LEU:HD11	1.99	0.62
1:A:191:HIS:CD2	1:A:192:SER:H	2.16	0.62
2:B:29:LEU:O	2:B:33:GLU:HG3	2.00	0.62
2:B:15:GLU:HG3	2:B:16:GLY:H	1.65	0.62
2:B:18:ARG:HB2	2:B:21:TYR:CE1	2.34	0.61
2:B:65:PHE:HZ	2:B:96:GLN:HB3	1.64	0.61
2:B:4:LEU:HG	2:B:8:GLN:OE1	1.99	0.61
2:B:6:PRO:CB	2:B:30:LEU:HD22	2.29	0.61
2:B:29:LEU:HG	2:B:33:GLU:CD	2.20	0.60
1:A:159:LEU:HD23	1:A:170:VAL:HG13	1.83	0.60
1:A:286:SER:HA	1:A:314:GLU:HB3	1.83	0.60
1:A:152:ARG:HD3	2:B:48:GLU:CG	2.26	0.60
2:B:18:ARG:HD3	2:B:135:VAL:HG23	1.83	0.60
2:B:34:SER:O	2:B:38:VAL:HG23	2.02	0.59
2:B:85:PRO:HG2	2:B:88:GLY:O	2.02	0.59
1:A:1:MET:HB3	1:A:66:GLY:CA	2.33	0.59
1:A:136:LYS:HG3	1:A:204:MET:HE2	1.84	0.59
2:B:117:LEU:HD22	2:B:122:GLU:CG	2.33	0.58
1:A:224:ARG:HD2	1:A:231:ILE:CG2	2.33	0.58
2:B:81:LEU:HD12	2:B:82:LEU:H	1.68	0.58
2:B:24:LEU:HD23	2:B:117:LEU:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HB	1:A:236:LEU:HD13	1.85	0.57
2:B:31:LEU:HD23	2:B:139:CYS:HB2	1.86	0.57
2:B:39:ARG:CZ	2:B:50:HIS:HB3	2.34	0.57
1:A:12:LYS:CB	1:A:13:PRO:HD3	2.35	0.57
1:A:362:MET:HG2	2:B:73:LEU:CD2	2.34	0.57
2:B:95:GLU:O	2:B:98:LEU:HB3	2.05	0.56
1:A:48:ASP:O	1:A:49:LEU:HB2	2.04	0.56
1:A:349:ILE:N	1:A:349:ILE:HD13	2.21	0.56
2:B:118:SER:HB2	2:B:121:GLN:CB	2.34	0.56
1:A:342:ASP:HB3	1:A:344:VAL:H	1.71	0.56
1:A:32:ASN:CB	1:A:69:THR:HG23	2.30	0.56
1:A:16:GLN:HG2	1:A:230:PHE:CD2	2.41	0.55
1:A:327:VAL:HG11	1:A:349:ILE:HB	1.88	0.55
1:A:18:SER:HB3	1:A:72:ALA:HB1	1.87	0.55
2:B:121:GLN:O	2:B:123:ASN:N	2.39	0.55
1:A:256:LEU:HB3	1:A:310:TYR:CD1	2.42	0.54
2:B:81:LEU:O	2:B:82:LEU:HD12	2.06	0.54
1:A:70:VAL:HG12	1:A:110:THR:HG22	1.90	0.54
2:B:84:LEU:HB2	2:B:113:ARG:O	2.07	0.54
2:B:18:ARG:CD	2:B:135:VAL:HG23	2.38	0.54
2:B:6:PRO:HG3	2:B:139:CYS:HA	1.89	0.54
2:B:5:TYR:N	2:B:8:GLN:OE1	2.41	0.54
1:A:33:LEU:HG	1:A:72:ALA:CB	2.38	0.54
2:B:86:GLU:CA	2:B:115:ASN:HD21	2.21	0.54
2:B:93:ILE:HG22	2:B:97:LEU:HD22	1.89	0.54
2:B:18:ARG:HG2	2:B:134:SER:HA	1.90	0.54
1:A:270:ALA:O	1:A:294:ALA:HB2	2.07	0.54
2:B:90:ASN:H	2:B:93:ILE:HD12	1.73	0.53
1:A:281:VAL:CG1	1:A:282:ARG:N	2.72	0.53
1:A:198:LYS:H	1:A:198:LYS:CD	2.20	0.52
1:A:256:LEU:HB3	1:A:310:TYR:HD1	1.75	0.52
2:B:120:ALA:O	2:B:123:ASN:OD1	2.26	0.52
2:B:55:ILE:HG22	2:B:93:ILE:HD13	1.91	0.52
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.91	0.52
1:A:153:TYR:HA	1:A:156:ASN:ND2	2.25	0.52
1:A:136:LYS:HG3	1:A:204:MET:HE1	1.89	0.52
1:A:342:ASP:HB2	1:A:345:SER:OG	2.09	0.52
2:B:100:LEU:O	2:B:100:LEU:HD23	2.08	0.52
1:A:130:LEU:H	1:A:130:LEU:HD12	1.75	0.52
2:B:48:GLU:CG	2:B:76:SER:HB2	2.23	0.52
1:A:288:ASN:HA	1:A:310:TYR:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:GLU:O	2:B:78:GLN:HA	2.10	0.51
1:A:215:ARG:HG3	1:A:215:ARG:O	2.09	0.51
1:A:97:MET:O	1:A:107:SER:HA	2.10	0.51
2:B:98:LEU:HA	2:B:126:TRP:HB3	1.92	0.51
2:B:6:PRO:CG	2:B:139:CYS:HA	2.41	0.51
1:A:123:GLN:HA	1:A:123:GLN:OE1	2.09	0.51
1:A:260:CYS:SG	1:A:264:LYS:HE2	2.50	0.51
1:A:10:LEU:O	1:A:14:LEU:HB2	2.11	0.51
1:A:177:LEU:HD11	1:A:244:TYR:HB2	1.93	0.51
2:B:124:ALA:CB	2:B:126:TRP:NE1	2.74	0.51
1:A:125:GLU:OE1	1:A:220:SER:HB3	2.11	0.50
2:B:13:LEU:HD21	2:B:38:VAL:HA	1.92	0.50
2:B:56:ASP:HB2	2:B:57:PRO:CD	2.36	0.50
1:A:260:CYS:HB2	1:A:336:VAL:HG23	1.94	0.50
1:A:282:ARG:HG3	1:A:366:LEU:HD11	1.93	0.50
1:A:7:ARG:HD2	1:A:82:LEU:HB2	1.93	0.50
2:B:25:GLY:H	2:B:115:ASN:HA	1.76	0.50
2:B:27:ASP:HB3	2:B:139:CYS:O	2.12	0.50
2:B:13:LEU:HD21	2:B:37:ALA:O	2.13	0.49
2:B:11:ALA:O	2:B:15:GLU:HG2	2.12	0.49
2:B:116:LYS:HE3	2:B:117:LEU:O	2.12	0.49
1:A:197:ARG:HB3	1:A:198:LYS:HE2	1.95	0.49
2:B:104:LEU:HD21	2:B:110:LEU:HB2	1.94	0.49
2:B:23:LEU:HD23	2:B:137:VAL:HB	1.94	0.49
2:B:80:LEU:HG	2:B:82:LEU:CD1	2.42	0.49
1:A:365:ARG:O	1:A:366:LEU:CB	2.60	0.48
2:B:23:LEU:CD2	2:B:137:VAL:HB	2.43	0.48
1:A:132:GLN:HG3	1:A:212:ASN:O	2.13	0.48
1:A:153:TYR:HA	1:A:156:ASN:HD22	1.79	0.48
1:A:305:ILE:HD12	1:A:305:ILE:N	2.29	0.48
1:A:208:ASP:C	1:A:210:GLY:H	2.16	0.48
2:B:22:LEU:HB3	2:B:24:LEU:CD1	2.44	0.48
2:B:51:HIS:CD2	2:B:67:LEU:HD11	2.49	0.48
2:B:55:ILE:CG2	2:B:93:ILE:HD13	2.44	0.48
2:B:117:LEU:HD23	2:B:118:SER:N	2.29	0.47
2:B:124:ALA:HB1	2:B:126:TRP:CD1	2.49	0.47
1:A:321:VAL:HG12	1:A:325:LEU:CD1	2.43	0.47
1:A:230:PHE:C	1:A:231:ILE:HG13	2.34	0.47
2:B:24:LEU:N	2:B:24:LEU:HD12	2.30	0.47
1:A:27:LEU:HG	1:A:28:PRO:HD2	1.95	0.47
2:B:38:VAL:O	2:B:42:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LEU:HB3	2:B:24:LEU:HD11	1.96	0.47
1:A:130:LEU:N	1:A:130:LEU:HD12	2.29	0.47
1:A:177:LEU:C	1:A:177:LEU:HD23	2.35	0.47
1:A:347:VAL:HG12	1:A:348:GLN:N	2.30	0.46
2:B:6:PRO:HB2	2:B:30:LEU:HD22	1.95	0.46
1:A:310:TYR:CG	1:A:311:SER:N	2.82	0.46
1:A:82:LEU:HD12	1:A:88:ILE:HD11	1.97	0.46
2:B:24:LEU:CD1	2:B:24:LEU:N	2.78	0.46
2:B:13:LEU:HD21	2:B:37:ALA:C	2.36	0.46
2:B:38:VAL:HG12	2:B:109:LEU:HD21	1.97	0.46
1:A:201:ILE:O	1:A:204:MET:HB3	2.16	0.46
1:A:214:LEU:HD12	1:A:215:ARG:N	2.31	0.46
1:A:365:ARG:O	1:A:366:LEU:HB3	2.16	0.46
2:B:92:ALA:C	2:B:94:ASN:N	2.70	0.46
2:B:124:ALA:HB1	2:B:126:TRP:NE1	2.31	0.46
2:B:98:LEU:CA	2:B:126:TRP:HB3	2.45	0.45
1:A:106:PHE:CD1	1:A:106:PHE:N	2.84	0.45
2:B:94:ASN:HB3	2:B:124:ALA:HB1	1.97	0.45
1:A:103:ARG:HA	1:A:103:ARG:HD3	1.47	0.45
1:A:218:ILE:CD1	1:A:218:ILE:N	2.78	0.45
1:A:342:ASP:HB2	1:A:345:SER:H	1.81	0.45
2:B:27:ASP:O	2:B:31:LEU:HG	2.17	0.45
2:B:55:ILE:HD11	2:B:82:LEU:HD23	1.99	0.45
1:A:40:GLY:O	1:A:59:LEU:N	2.34	0.45
2:B:18:ARG:HD3	2:B:135:VAL:CG2	2.46	0.45
1:A:137:ARG:HH11	1:A:137:ARG:HG3	1.81	0.45
1:A:2:LYS:HB3	1:A:64:GLU:HB3	1.98	0.45
2:B:139:CYS:O	2:B:140:GLN:O	2.34	0.45
2:B:48:GLU:CD	2:B:76:SER:HB3	2.37	0.45
2:B:67:LEU:O	2:B:67:LEU:HD23	2.17	0.44
2:B:115:ASN:O	2:B:116:LYS:C	2.55	0.44
2:B:42:ALA:O	2:B:44:ALA:N	2.51	0.44
1:A:144:PHE:CE1	1:A:326:ASP:HB3	2.53	0.44
1:A:44:LEU:CD1	1:A:44:LEU:N	2.79	0.44
2:B:10:ARG:O	2:B:14:ASN:HB2	2.17	0.44
2:B:25:GLY:O	2:B:31:LEU:HD21	2.17	0.44
2:B:31:LEU:HD23	2:B:139:CYS:CB	2.48	0.44
2:B:93:ILE:O	2:B:97:LEU:HB2	2.17	0.44
2:B:122:GLU:H	2:B:122:GLU:HG3	1.50	0.44
2:B:22:LEU:CD2	2:B:22:LEU:N	2.80	0.44
2:B:94:ASN:HA	2:B:126:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:HA	2:B:111:ILE:O	2.18	0.44
2:B:79:THR:O	2:B:79:THR:HG22	2.18	0.44
2:B:82:LEU:HD13	2:B:110:LEU:HD11	1.99	0.44
2:B:32:GLN:O	2:B:35:GLN:HG2	2.18	0.44
1:A:16:GLN:HG2	1:A:230:PHE:CE2	2.53	0.44
2:B:4:LEU:CD2	2:B:12:GLN:CG	2.85	0.44
1:A:281:VAL:HG13	1:A:282:ARG:N	2.32	0.43
1:A:249:PRO:HD3	1:A:346:SER:OG	2.18	0.43
2:B:116:LYS:HD2	2:B:117:LEU:N	2.32	0.43
2:B:20:ALA:HB3	2:B:134:SER:CB	2.40	0.43
1:A:121:ASP:OD1	1:A:122:TRP:N	2.52	0.43
1:A:170:VAL:HG22	1:A:241:PHE:CE2	2.53	0.43
2:B:65:PHE:O	2:B:69:GLN:HG2	2.18	0.43
2:B:78:GLN:H	2:B:78:GLN:HG2	1.66	0.43
1:A:64:GLU:HA	1:A:65:PRO:HD2	1.90	0.43
1:A:204:MET:HA	1:A:204:MET:HE3	2.01	0.43
1:A:48:ASP:O	1:A:49:LEU:CB	2.67	0.42
2:B:80:LEU:HB3	2:B:108:LEU:HD11	2.01	0.42
1:A:176:ARG:HG2	1:A:176:ARG:NH1	2.33	0.42
2:B:42:ALA:O	2:B:43:ALA:C	2.57	0.42
2:B:42:ALA:C	2:B:44:ALA:N	2.73	0.42
1:A:254:LYS:C	1:A:255:HIS:HD2	2.23	0.42
1:A:26:THR:OG1	1:A:30:LEU:HD12	2.19	0.42
2:B:9:LEU:CD2	2:B:34:SER:HA	2.50	0.41
2:B:34:SER:O	2:B:37:ALA:HB3	2.21	0.41
1:A:208:ASP:O	1:A:210:GLY:N	2.45	0.41
1:A:279:ARG:HD3	1:A:279:ARG:HA	1.88	0.41
1:A:286:SER:O	1:A:287:GLU:C	2.58	0.41
1:A:39:ASP:O	1:A:41:THR:N	2.54	0.41
2:B:92:ALA:C	2:B:94:ASN:H	2.22	0.41
1:A:191:HIS:CD2	1:A:192:SER:N	2.86	0.41
2:B:24:LEU:CD2	2:B:117:LEU:HB2	2.50	0.41
2:B:98:LEU:C	2:B:98:LEU:HD13	2.41	0.41
2:B:118:SER:CB	2:B:121:GLN:CG	2.97	0.41
2:B:81:LEU:HG	2:B:82:LEU:N	2.36	0.41
1:A:261:ASP:O	1:A:265:GLN:HG3	2.21	0.41
1:A:282:ARG:HD3	1:A:316:GLU:OE1	2.21	0.41
1:A:260:CYS:SG	1:A:264:LYS:CE	3.09	0.41
2:B:118:SER:HB2	2:B:121:GLN:CG	2.51	0.41
2:B:4:LEU:HG	2:B:8:GLN:CD	2.40	0.41
1:A:40:GLY:O	1:A:59:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:SER:CB	1:A:72:ALA:HB1	2.49	0.40
2:B:123:ASN:O	2:B:124:ALA:C	2.59	0.40
2:B:61:TRP:HE3	2:B:65:PHE:CE2	2.39	0.40
1:A:17:VAL:HG23	1:A:18:SER:N	2.36	0.40
1:A:284:TYR:HB3	1:A:291:LYS:HB2	2.04	0.40
2:B:118:SER:HB2	2:B:121:GLN:HG3	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	364/366 (100%)	333 (92%)	26 (7%)	5 (1%)	13	23
2	B	138/140 (99%)	115 (83%)	18 (13%)	5 (4%)	4	5
All	All	502/506 (99%)	448 (89%)	44 (9%)	10 (2%)	9	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLY
2	B	119	LYS
2	B	122	GLU
2	B	131	ALA
1	A	40	GLY
1	A	121	ASP
2	B	118	SER
1	A	332	LYS
2	B	43	ALA
1	A	209	GLY

### 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	311/311 (100%)	293 (94%)	18 (6%)	23	43
2	B	117/117 (100%)	111 (95%)	6 (5%)	28	50
All	All	428/428 (100%)	404 (94%)	24 (6%)	25	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	39	ASP
1	A	41	THR
1	A	73	ARG
1	A	107	SER
1	A	120	ASP
1	A	123	GLN
1	A	130	LEU
1	A	135	MET
1	A	170	VAL
1	A	176	ARG
1	A	198	LYS
1	A	215	ARG
1	A	256	LEU
1	A	261	ASP
1	A	275	ASN
1	A	276	GLU
1	A	340	LEU
2	B	4	LEU
2	B	8	GLN
2	B	78	GLN
2	B	106	ASP
2	B	115	ASN
2	B	123	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	191	HIS
1	A	255	HIS
1	A	329	ASN
2	B	78	GLN
2	B	115	ASN
2	B	123	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	366/366 (100%)	0.36	19 (5%)	28 29	27, 49, 93, 123	0
2	B	140/140 (100%)	1.81	51 (36%)	0 0	50, 123, 144, 150	0
All	All	506/506 (100%)	0.76	70 (13%)	3 3	27, 58, 134, 150	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	GLY	8.5
2	B	140	GLN	7.5
2	B	13	LEU	6.1
2	B	21	TYR	6.0
2	B	10	ARG	5.4
2	B	17	LEU	5.3
2	B	23	LEU	5.1
2	B	119	LYS	5.1
2	B	91	ALA	5.0
2	B	26	ASN	5.0
2	B	1	MET	4.8
1	A	20	PRO	4.6
1	A	312	GLY	4.6
1	A	19	GLY	4.6
2	B	90	ASN	4.6
2	B	14	ASN	4.6
1	A	21	LEU	4.5
2	B	18	ARG	4.4
2	B	86	GLU	4.4
1	A	22	GLY	4.3
2	B	124	ALA	4.3
1	A	301	GLU	4.2
1	A	209	GLY	4.2
2	B	131	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	298	GLU	4.1
2	B	112	VAL	4.1
1	A	24	ARG	3.9
1	A	297	PRO	3.8
2	B	92	ALA	3.7
2	B	58	ASN	3.6
2	B	133	ARG	3.6
1	A	299	GLN	3.6
2	B	30	LEU	3.6
2	B	4	LEU	3.5
2	B	123	ASN	3.4
2	B	120	ALA	3.4
2	B	3	ARG	3.3
2	B	16	GLY	3.3
2	B	43	ALA	3.2
2	B	12	GLN	3.1
2	B	117	LEU	3.0
2	B	111	ILE	3.0
2	B	59	THR	2.9
1	A	210	GLY	2.8
2	B	110	LEU	2.8
2	B	20	ALA	2.8
2	B	132	ASN	2.8
2	B	46	GLY	2.7
2	B	9	LEU	2.7
2	B	87	ASN	2.7
2	B	76	SER	2.6
1	A	25	PRO	2.5
1	A	300	GLU	2.5
2	B	22	LEU	2.5
2	B	57	PRO	2.5
2	B	135	VAL	2.4
2	B	25	GLY	2.4
2	B	50	HIS	2.3
2	B	28	PRO	2.3
2	B	2	ILE	2.3
2	B	88	GLY	2.3
1	A	169	THR	2.3
1	A	353	ALA	2.2
1	A	17	VAL	2.2
2	B	122	GLU	2.1
2	B	137	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	ARG	2.1
2	B	89	PRO	2.1
2	B	77	ARG	2.0
2	B	116	LYS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.