



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2021 – 12:07 PM JST

PDB ID : 7DEY  
Title : Structure of Dicer from *Pichia stipitis*  
Authors : Jobichen, C.; Jingru, C.  
Deposited on : 2020-11-05  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

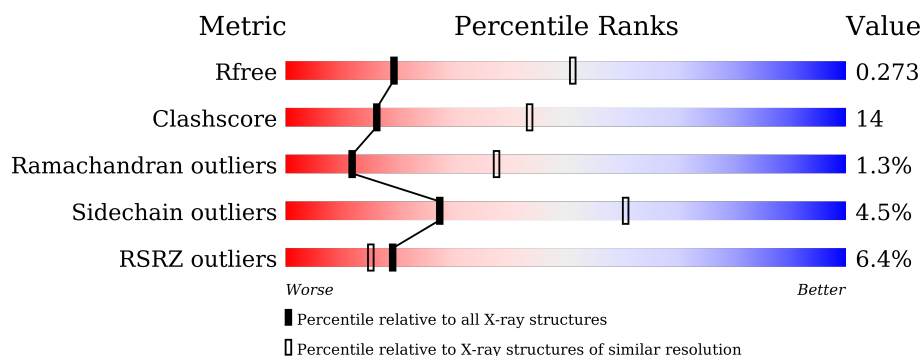
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	231	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>27%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	231	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div></div> <div>10%</div> </div> </div>
1	D	231	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>22%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6267 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.

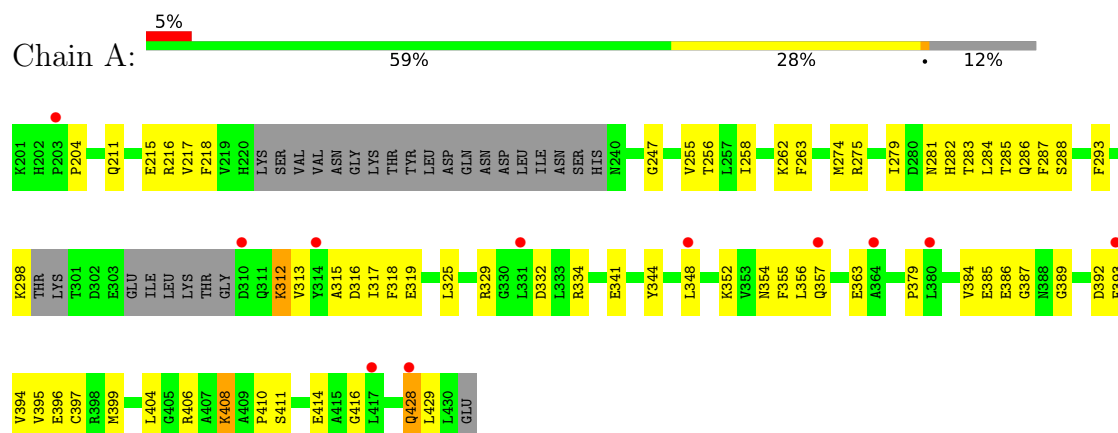
- Molecule 1 is a protein called RNase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1578	1011	268	295	4			
1	B	199	Total	C	N	O	S	0	0	0
			1520	971	260	285	4			
1	C	207	Total	C	N	O	S	0	0	0
			1593	1018	272	299	4			
1	D	207	Total	C	N	O	S	0	0	0
			1576	1006	270	297	3			

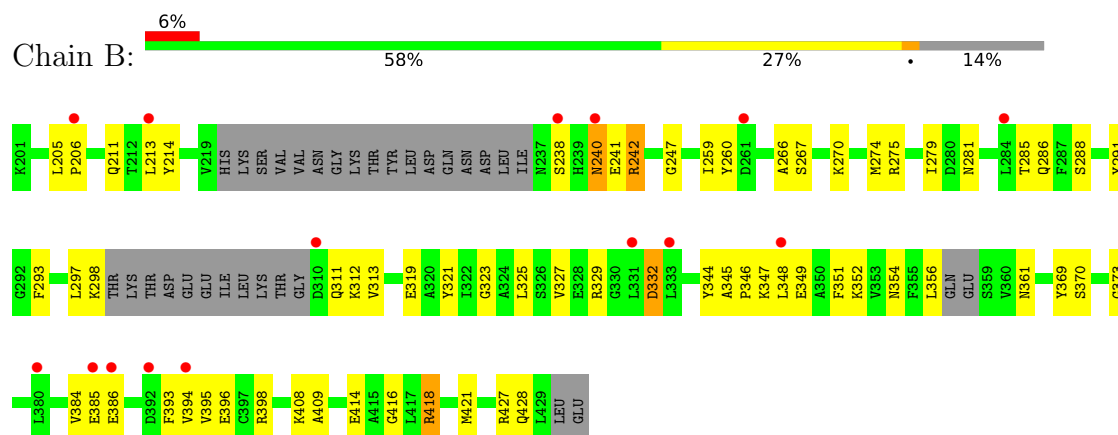
### 3 Residue-property plots [i](#)

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.

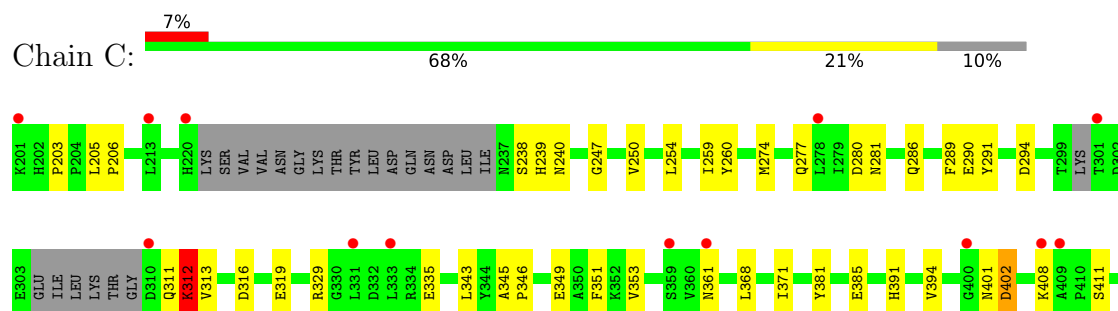
#### • Molecule 1: RNase III

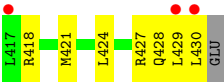


#### • Molecule 1: RNase III

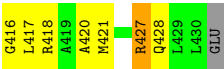
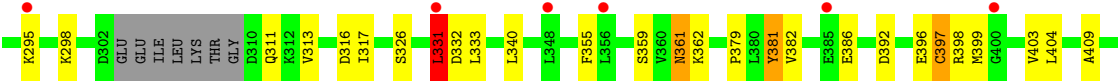


#### • Molecule 1: RNase III





● Molecule 1: RNase III



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.74Å 127.74Å 103.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.90 29.68 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.68-2.90) 99.1 (29.68-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.97 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, $R_{free}$	0.235 , 0.272 0.238 , 0.273	Depositor DCC
$R_{free}$ test set	2016 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% 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	0.47	0/1605	0.65	0/2164
1	B	0.47	0/1545	0.62	0/2086
1	C	0.46	0/1620	0.60	0/2186
1	D	0.49	0/1603	0.71	0/2165
All	All	0.47	0/6373	0.65	0/8601

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	1578	0	1535	51	0
1	B	1520	0	1470	58	0
1	C	1593	0	1540	35	0
1	D	1576	0	1531	48	0
All	All	6267	0	6076	178	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 14.

All (178) 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:414:GLU:O	1:B:418:ARG:HD3	1.50	1.09
1:B:409:ALA:CB	1:B:418:ARG:HH21	1.76	0.99
1:B:409:ALA:HB2	1:B:418:ARG:HE	1.30	0.92
1:D:267:SER:H	1:D:270:LYS:HE3	1.36	0.90
1:B:267:SER:H	1:B:270:LYS:HE2	1.38	0.88
1:D:255:VAL:HG21	1:D:279:ILE:HD11	1.55	0.87
1:D:381:TYR:OH	1:D:420:ALA:HB2	1.74	0.86
1:B:409:ALA:CB	1:B:418:ARG:NH2	2.42	0.83
1:B:395:VAL:HG21	1:B:416:GLY:HA2	1.59	0.83
1:B:409:ALA:HB2	1:B:418:ARG:NE	1.93	0.82
1:A:255:VAL:HG21	1:A:279:ILE:HD11	1.63	0.81
1:B:347:LYS:HD2	1:B:347:LYS:H	1.47	0.79
1:A:282:HIS:O	1:A:285:THR:HG22	1.85	0.77
1:B:409:ALA:HB2	1:B:418:ARG:HH21	1.49	0.75
1:A:394:VAL:HG12	1:A:408:LYS:HB3	1.69	0.75
1:D:266:ALA:HB1	1:D:270:LYS:HG3	1.69	0.74
1:B:311:GLN:HG3	1:B:313:VAL:H	1.54	0.73
1:B:409:ALA:HB2	1:B:418:ARG:NH2	2.05	0.72
1:A:392:ASP:OD2	1:A:410:PRO:HA	1.91	0.71
1:C:329:ARG:NE	1:C:335:GLU:OE1	2.22	0.71
1:A:263:PHE:CE1	1:A:352:LYS:HB2	2.27	0.70
1:D:397:CYS:SG	1:D:404:LEU:HB2	2.32	0.70
1:A:379:PRO:HB3	1:A:399:MET:HE2	1.74	0.69
1:B:409:ALA:CA	1:B:418:ARG:HH21	2.06	0.68
1:D:379:PRO:HA	1:D:399:MET:HA	1.77	0.66
1:A:344:TYR:HB3	1:A:348:LEU:HD13	1.77	0.66
1:D:259:ILE:HD12	1:D:274:MET:HG3	1.78	0.66
1:C:418:ARG:HG2	1:C:421:MET:HE3	1.77	0.66
1:A:263:PHE:HE1	1:A:352:LYS:HB2	1.61	0.65
1:D:381:TYR:H	1:D:381:TYR:HD1	1.43	0.64
1:C:312:LYS:H	1:C:312:LYS:HD2	1.63	0.63
1:C:394:VAL:HG12	1:C:408:LYS:HB3	1.79	0.63
1:C:274:MET:HG2	1:C:351:PHE:HD2	1.63	0.63
1:B:409:ALA:HB2	1:B:418:ARG:CZ	2.27	0.63
1:C:329:ARG:HE	1:C:335:GLU:CD	2.01	0.63
1:B:275:ARG:O	1:B:279:ILE:HG12	1.98	0.62
1:C:430:LEU:HD12	1:C:430:LEU:H	1.64	0.62
1:C:385:GLU:HB3	1:C:394:VAL:HG22	1.84	0.60
1:D:362:LYS:HA	1:D:417:LEU:HD13	1.82	0.60
1:B:325:LEU:O	1:B:329:ARG:HD2	2.01	0.59
1:B:427:ARG:HB3	1:D:211:GLN:NE2	2.17	0.59
1:B:344:TYR:HA	1:B:347:LYS:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:LYS:HA	1:D:295:LYS:HE2	1.85	0.59
1:B:409:ALA:HA	1:B:418:ARG:HH21	1.66	0.58
1:C:205:LEU:HB2	1:C:291:TYR:CE1	2.38	0.58
1:B:414:GLU:HG2	1:B:418:ARG:HD2	1.86	0.58
1:A:204:PRO:HB3	1:C:361:ASN:H	1.68	0.58
1:B:385:GLU:HG3	1:B:394:VAL:HB	1.86	0.57
1:B:361:ASN:HB3	1:B:421:MET:SD	2.45	0.57
1:D:359:SER:O	1:D:418:ARG:NH2	2.37	0.57
1:A:352:LYS:O	1:A:352:LYS:HE3	2.05	0.56
1:B:323:GLY:O	1:B:327:VAL:HG23	2.04	0.56
1:A:385:GLU:HB2	1:A:394:VAL:CG2	2.36	0.56
1:C:402:ASP:OD1	1:C:402:ASP:N	2.26	0.56
1:D:267:SER:N	1:D:270:LYS:HE3	2.14	0.56
1:D:331:LEU:HD13	1:D:331:LEU:N	2.20	0.55
1:D:381:TYR:CD1	1:D:381:TYR:N	2.74	0.55
1:B:409:ALA:HB1	1:B:418:ARG:NH2	2.22	0.55
1:A:283:THR:HA	1:A:286:GLN:HG2	1.89	0.55
1:B:286:GLN:OE1	1:D:277:GLN:NE2	2.30	0.55
1:C:349:GLU:O	1:C:353:VAL:HG23	2.06	0.55
1:A:312:LYS:HE3	1:A:316:ASP:OD2	2.06	0.55
1:C:274:MET:HG2	1:C:351:PHE:CD2	2.42	0.55
1:C:247:GLY:HA3	1:C:319:GLU:O	2.07	0.55
1:A:313:VAL:O	1:A:317:ILE:HD12	2.07	0.54
1:A:385:GLU:HB2	1:A:394:VAL:HG22	1.89	0.54
1:B:414:GLU:HG2	1:B:418:ARG:CD	2.36	0.54
1:B:394:VAL:HG22	1:B:408:LYS:HB3	1.90	0.54
1:A:386:GLU:HA	1:A:393:PHE:HD1	1.73	0.54
1:B:393:PHE:O	1:B:408:LYS:HA	2.08	0.53
1:B:266:ALA:HA	1:B:270:LYS:HE3	1.90	0.53
1:A:411:SER:HB3	1:A:414:GLU:H	1.73	0.53
1:C:281:ASN:ND2	1:C:312:LYS:HB3	2.24	0.53
1:B:427:ARG:HB3	1:D:211:GLN:HE22	1.74	0.52
1:A:258:ILE:HG12	1:A:341:GLU:HG3	1.91	0.52
1:D:326:SER:HB3	1:D:333:LEU:CD2	2.40	0.52
1:A:247:GLY:HA3	1:A:319:GLU:O	2.09	0.52
1:A:211:GLN:O	1:A:215:GLU:HG3	2.11	0.51
1:D:205:LEU:HB2	1:D:291:TYR:CD1	2.45	0.51
1:A:262:LYS:HD2	1:A:262:LYS:N	2.26	0.51
1:A:356:LEU:HG	1:A:357:GLN:HG2	1.93	0.51
1:A:281:ASN:HD22	1:A:312:LYS:HA	1.76	0.50
1:A:395:VAL:HG21	1:A:416:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LEU:HD12	1:C:206:PRO:HD2	1.94	0.50
1:D:399:MET:CB	1:D:404:LEU:HD11	2.41	0.50
1:D:259:ILE:HG13	1:D:271:LEU:HD22	1.92	0.50
1:D:311:GLN:HB3	1:D:313:VAL:HG12	1.94	0.50
1:A:386:GLU:HA	1:A:393:PHE:CD1	2.47	0.50
1:A:357:GLN:HE22	1:C:286:GLN:HG3	1.76	0.49
1:C:371:ILE:HD13	1:C:427:ARG:HD3	1.94	0.49
1:A:394:VAL:CG1	1:A:408:LYS:HB3	2.39	0.49
1:B:211:GLN:HA	1:D:427:ARG:NH2	2.27	0.49
1:A:284:LEU:HD11	1:A:318:PHE:CD2	2.48	0.48
1:C:313:VAL:O	1:C:316:ASP:N	2.46	0.48
1:C:394:VAL:HG12	1:C:408:LYS:CB	2.43	0.48
1:B:241:GLU:O	1:B:242:ARG:HB3	2.14	0.48
1:B:247:GLY:HA3	1:B:319:GLU:O	2.12	0.48
1:D:382:VAL:HG21	1:D:398:ARG:NH2	2.29	0.48
1:A:256:THR:OG1	1:A:275:ARG:HD3	2.14	0.48
1:A:274:MET:HE2	1:A:274:MET:HB3	1.54	0.48
1:C:345:ALA:HB3	1:C:346:PRO:HD3	1.95	0.48
1:A:387:GLY:O	1:A:389:GLY:N	2.47	0.47
1:C:428:GLN:NE2	1:C:429:LEU:H	2.12	0.47
1:D:298:LYS:HD3	1:D:298:LYS:HA	1.69	0.47
1:A:217:VAL:HG13	1:A:218:PHE:CD2	2.48	0.47
1:A:379:PRO:CB	1:A:399:MET:HE2	2.44	0.47
1:D:428:GLN:N	1:D:428:GLN:OE1	2.47	0.47
1:A:355:PHE:CD1	1:A:355:PHE:O	2.68	0.47
1:B:332:ASP:OD2	1:B:332:ASP:N	2.47	0.47
1:B:354:ASN:O	1:B:356:LEU:N	2.44	0.47
1:C:368:LEU:HA	1:C:424:LEU:HD21	1.95	0.47
1:B:205:LEU:HB2	1:B:291:TYR:CD1	2.49	0.47
1:C:385:GLU:HB3	1:C:394:VAL:CG2	2.44	0.47
1:D:210:ASP:HB3	1:D:213:LEU:HB2	1.97	0.47
1:D:404:LEU:HD12	1:D:404:LEU:H	1.80	0.47
1:B:274:MET:HG2	1:B:351:PHE:CD2	2.50	0.47
1:C:203:PRO:HG3	1:C:343:LEU:HA	1.97	0.46
1:A:329:ARG:HD3	1:A:332:ASP:O	2.16	0.46
1:A:282:HIS:HD2	1:C:280:ASP:OD2	1.98	0.46
1:A:288:SER:O	1:A:293:PHE:HB2	2.15	0.46
1:A:363:GLU:N	1:A:363:GLU:OE2	2.47	0.46
1:C:286:GLN:HG2	1:C:290:GLU:OE2	2.15	0.45
1:D:279:ILE:O	1:D:279:ILE:HG22	2.17	0.45
1:A:284:LEU:HD11	1:A:318:PHE:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:PRO:O	1:B:321:TYR:OH	2.29	0.45
1:D:266:ALA:HB1	1:D:270:LYS:CG	2.42	0.45
1:D:274:MET:O	1:D:278:LEU:HG	2.17	0.45
1:D:254:LEU:O	1:D:258:ILE:HG13	2.16	0.45
1:D:379:PRO:O	1:D:398:ARG:O	2.35	0.45
1:C:368:LEU:HD23	1:C:381:TYR:OH	2.17	0.45
1:D:281:ASN:O	1:D:285:THR:HG23	2.17	0.45
1:A:325:LEU:O	1:A:329:ARG:HG2	2.17	0.45
1:D:392:ASP:HB3	1:D:409:ALA:O	2.18	0.44
1:B:297:LEU:C	1:B:298:LYS:HD2	2.38	0.44
1:D:361:ASN:HB3	1:D:421:MET:SD	2.57	0.44
1:A:284:LEU:HA	1:A:284:LEU:HD12	1.54	0.44
1:B:428:GLN:OE1	1:B:428:GLN:N	2.51	0.44
1:B:349:GLU:OE1	1:B:352:LYS:NZ	2.29	0.44
1:B:396:GLU:OE1	1:B:398:ARG:NE	2.48	0.44
1:B:409:ALA:CB	1:B:418:ARG:CZ	2.91	0.44
1:A:286:GLN:HB3	1:C:277:GLN:OE1	2.18	0.43
1:B:427:ARG:HD3	1:D:214:TYR:CE2	2.53	0.43
1:B:214:TYR:CE1	1:D:427:ARG:HD3	2.52	0.43
1:B:281:ASN:ND2	1:B:312:LYS:HD3	2.34	0.43
1:B:384:VAL:O	1:B:385:GLU:HG2	2.18	0.43
1:B:369:TYR:O	1:B:373:GLY:N	2.48	0.43
1:C:311:GLN:C	1:C:313:VAL:H	2.21	0.43
1:B:211:GLN:HA	1:D:427:ARG:HH21	1.83	0.43
1:D:396:GLU:HB2	1:D:403:VAL:HG23	1.99	0.43
1:A:279:ILE:HG22	1:A:279:ILE:O	2.18	0.43
1:C:250:VAL:O	1:C:254:LEU:HG	2.18	0.43
1:A:428:GLN:H	1:A:428:GLN:HG2	1.37	0.43
1:D:340:LEU:HD23	1:D:340:LEU:HA	1.84	0.43
1:A:286:GLN:HG3	1:A:287:PHE:N	2.34	0.42
1:C:259:ILE:HG13	1:C:260:TYR:N	2.34	0.42
1:D:381:TYR:CE2	1:D:416:GLY:O	2.72	0.42
1:B:259:ILE:HG13	1:B:260:TYR:N	2.35	0.42
1:B:344:TYR:O	1:B:348:LEU:HG	2.18	0.42
1:A:285:THR:HG21	1:C:277:GLN:HE22	1.84	0.42
1:B:281:ASN:O	1:B:285:THR:OG1	2.26	0.42
1:B:352:LYS:HE3	1:B:352:LYS:HB2	1.65	0.42
1:B:298:LYS:HG3	1:D:428:GLN:HE22	1.84	0.42
1:C:289:PHE:HE1	1:C:294:ASP:HB3	1.85	0.42
1:D:317:ILE:H	1:D:317:ILE:HD12	1.84	0.42
1:C:401:ASN:OD1	1:C:401:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:CYS:SG	1:A:404:LEU:HD12	2.59	0.42
1:D:213:LEU:HA	1:D:213:LEU:HD23	1.81	0.41
1:A:284:LEU:HD23	1:A:315:ALA:HB1	2.01	0.41
1:A:384:VAL:O	1:A:385:GLU:HG2	2.20	0.41
1:D:278:LEU:O	1:D:279:ILE:HD13	2.21	0.41
1:B:288:SER:HB3	1:B:293:PHE:CD2	2.55	0.41
1:A:396:GLU:HG2	1:A:406:ARG:HB3	2.02	0.41
1:B:409:ALA:CB	1:B:418:ARG:HE	2.16	0.41
1:B:345:ALA:HB3	1:B:346:PRO:HD3	2.03	0.41
1:B:427:ARG:HE	1:D:211:GLN:HE22	1.69	0.40
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.74	0.40
1:A:298:LYS:HA	1:A:298:LYS:HD3	1.98	0.40
1:D:313:VAL:O	1:D:317:ILE:HD12	2.22	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	195/231 (84%)	175 (90%)	18 (9%)	2 (1%)	15	45
1	B	191/231 (83%)	175 (92%)	15 (8%)	1 (0%)	29	61
1	C	199/231 (86%)	177 (89%)	20 (10%)	2 (1%)	15	45
1	D	201/231 (87%)	179 (89%)	17 (8%)	5 (2%)	5	21
All	All	786/924 (85%)	706 (90%)	70 (9%)	10 (1%)	12	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	429	LEU

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Mol	Chain	Res	Type
1	C	391	HIS
1	B	240	ASN
1	D	242	ARG
1	D	332	ASP
1	C	312	LYS
1	D	361	ASN
1	D	331	LEU
1	D	386	GLU

### 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	162/204 (79%)	157 (97%)	5 (3%)	40	74
1	B	154/204 (76%)	147 (96%)	7 (4%)	27	61
1	C	162/204 (79%)	156 (96%)	6 (4%)	34	68
1	D	162/204 (79%)	151 (93%)	11 (7%)	16	42
All	All	640/816 (78%)	611 (96%)	29 (4%)	27	61

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

Mol	Chain	Res	Type
1	A	216	ARG
1	A	312	LYS
1	A	334	ARG
1	A	408	LYS
1	A	428	GLN
1	B	238	SER
1	B	240	ASN
1	B	242	ARG
1	B	332	ASP
1	B	370	SER
1	B	386	GLU
1	B	418	ARG
1	C	238	SER

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Mol	Chain	Res	Type
1	C	239	HIS
1	C	240	ASN
1	C	312	LYS
1	C	402	ASP
1	C	411	SER
1	D	213	LEU
1	D	237	ASN
1	D	241	GLU
1	D	270	LYS
1	D	276	SER
1	D	316	ASP
1	D	331	LEU
1	D	355	PHE
1	D	381	TYR
1	D	397	CYS
1	D	427	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	277	GLN
1	D	237	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 monosaccharides 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	203/231 (87%)	0.69	11 (5%)	25 22	48, 71, 108, 140	0
1	B	199/231 (86%)	0.70	15 (7%)	14 11	48, 68, 105, 138	0
1	C	207/231 (89%)	0.66	16 (7%)	13 10	45, 74, 120, 142	0
1	D	207/231 (89%)	0.63	10 (4%)	30 27	44, 71, 119, 137	0
All	All	816/924 (88%)	0.67	52 (6%)	19 15	44, 71, 118, 142	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ASN	5.5
1	C	301	THR	4.3
1	B	310	ASP	4.2
1	C	417	LEU	4.0
1	D	201	LYS	3.9
1	C	361	ASN	3.5
1	B	380	LEU	3.5
1	D	356	LEU	3.4
1	A	428	GLN	3.4
1	B	331	LEU	3.3
1	D	331	LEU	3.3
1	D	245	PHE	3.2
1	D	400	GLY	3.1
1	B	238	SER	3.1
1	A	357	GLN	3.1
1	C	333	LEU	2.9
1	A	331	LEU	2.9
1	B	261	ASP	2.9
1	B	386	GLU	2.9
1	A	310	ASP	2.8
1	C	201	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	400	GLY	2.8
1	C	359	SER	2.6
1	D	213	LEU	2.6
1	D	385	GLU	2.5
1	C	220	HIS	2.4
1	B	392	ASP	2.4
1	A	314	TYR	2.4
1	C	429	LEU	2.4
1	C	278	LEU	2.4
1	B	385	GLU	2.3
1	A	364	ALA	2.3
1	A	393	PHE	2.3
1	A	203	PRO	2.2
1	B	206	PRO	2.2
1	B	333	LEU	2.2
1	D	295	LYS	2.2
1	A	348	LEU	2.2
1	B	348	LEU	2.2
1	C	331	LEU	2.2
1	C	430	LEU	2.2
1	B	213	LEU	2.1
1	A	417	LEU	2.1
1	C	310	ASP	2.1
1	D	348	LEU	2.1
1	C	408	LYS	2.1
1	C	409	ALA	2.1
1	B	394	VAL	2.1
1	D	218	PHE	2.0
1	B	284	LEU	2.0
1	A	380	LEU	2.0
1	C	213	LEU	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 monosaccharides 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.