



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:41 PM UTC

PDB ID : 7DEY / pdb_00007dey
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

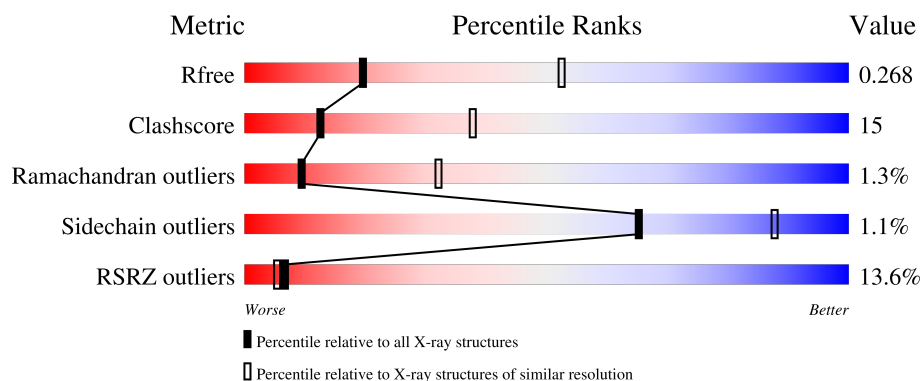
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 ≥ 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	11% 58% 29% 12%
1	B	231	13% 58% 28% 14%
1	C	231	11% 68% 21% 10%
1	D	231	13% 66% 23% 10%

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.

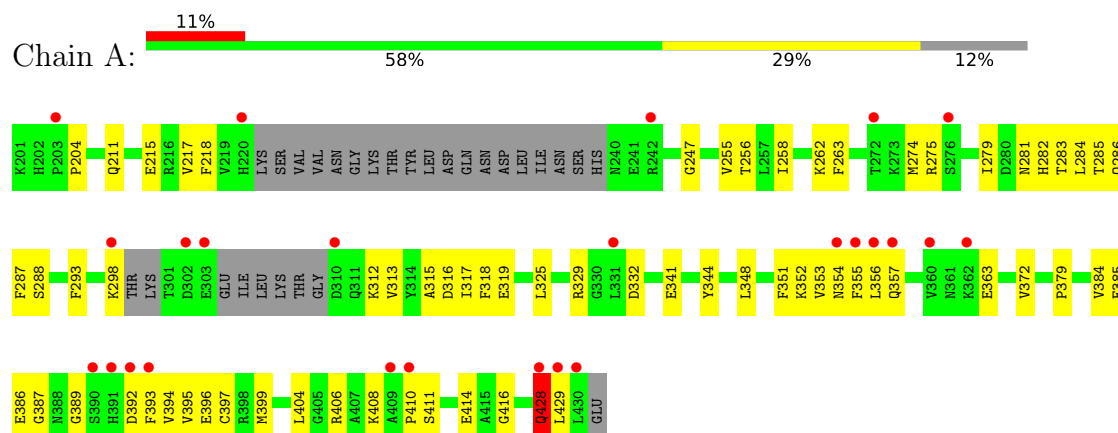
- Molecule 1 is a protein called RNase III.

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			

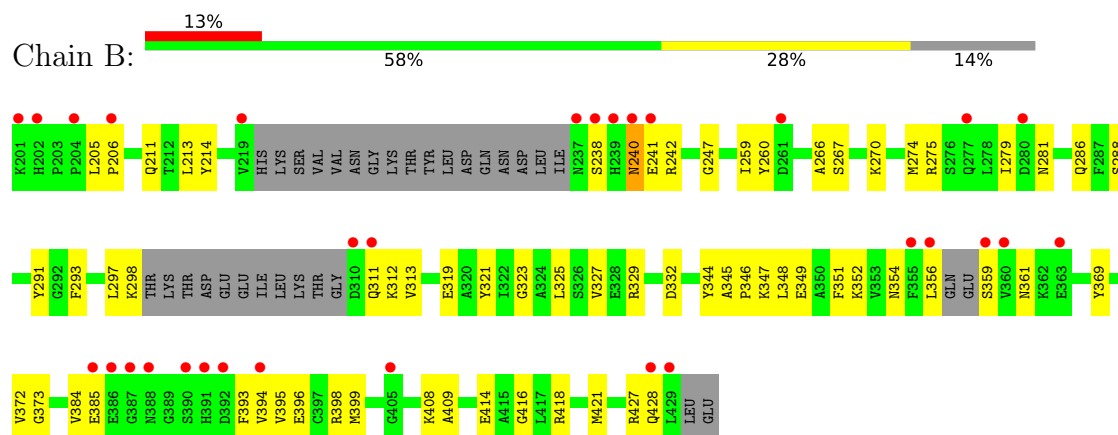
3 Residue-property plots [i](#)

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.

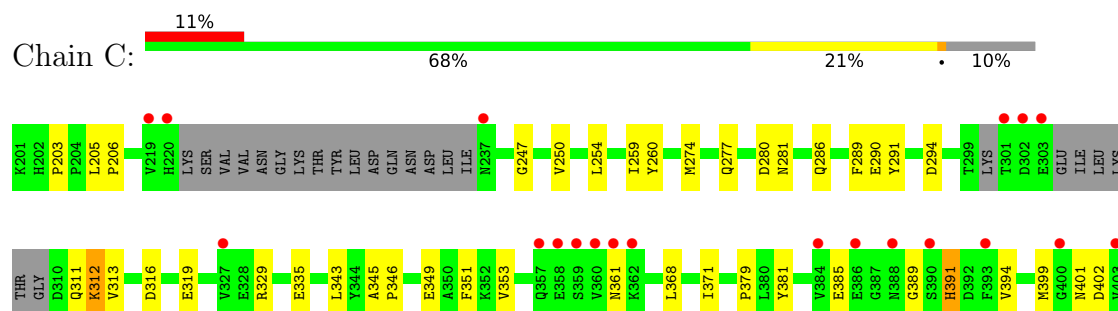
• Molecule 1: RNase III

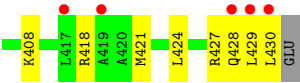


• Molecule 1: RNase III

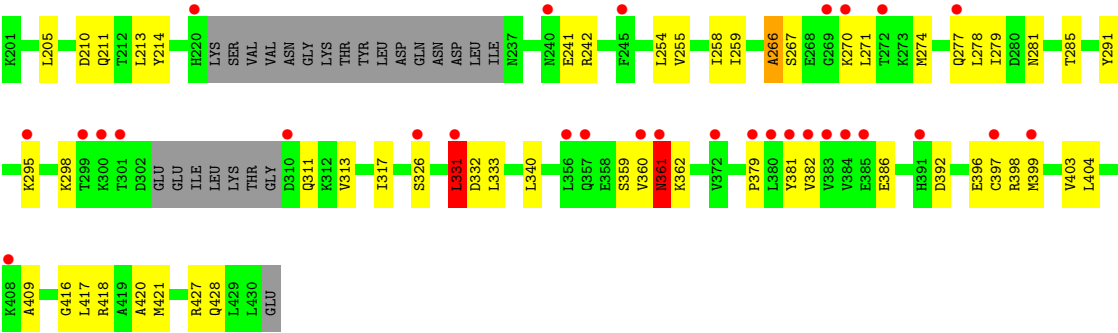


• Molecule 1: RNase III





● Molecule 1: RNase III



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	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) 99.0 (29.68-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.235 , 0.272 0.237 , 0.268	Depositor DCC
R_{free} test set	2016 reflections (5.43%)	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.44	0/1605	0.70	1/2164 (0.0%)
1	B	0.42	0/1545	0.66	0/2086
1	C	0.39	0/1620	0.66	0/2186
1	D	0.47	0/1603	0.81	4/2165 (0.2%)
All	All	0.43	0/6373	0.71	5/8601 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	ALA	O-C-N	-6.16	116.02	123.16
1	D	361	ASN	N-CA-C	5.94	123.44	110.80
1	D	360	VAL	CA-C-N	5.62	132.28	121.54
1	D	360	VAL	C-N-CA	5.62	132.28	121.54
1	A	428	GLN	N-CA-C	-5.21	105.24	111.03

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	56	0
1	B	1520	0	1470	58	0
1	C	1593	0	1540	40	0
1	D	1576	0	1531	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6267	0	6076	189	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 15.

All (189) 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:A:274:MET:HE3	1:A:351:PHE:HD2	1.45	0.80
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:B:409:ALA:CA	1:B:418:ARG:HH21	2.06	0.68
1:C:329:ARG:HE	1:C:335:GLU:CD	2.01	0.67
1:D:379:PRO:HA	1:D:399:MET:HA	1.77	0.66
1:A:263:PHE:CE2	1:A:274:MET:HE1	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:418:ARG:HA	1:C:421:MET:HE3	1.82	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
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:A:372:VAL:HG23	1:A:399:MET:HE1	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:297:LEU:C	1:B:298:LYS:HD2	2.38	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:B:372:VAL:O	1:B:399:MET:HE1	2.13	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:C:311:GLN:C	1:C:313:VAL:H	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:379:PRO:CD	1:A:399:MET:HE2	2.45	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:A:274:MET:HE2	1:A:274:MET:HB3	1.50	0.45
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
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:C:428:GLN:CD	1:C:429:LEU:N	2.76	0.44
1:D:392:ASP:HB3	1:D:409:ALA:O	2.18	0.44
1:A:363:GLU:H	1:A:363:GLU:CD	2.26	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:428:GLN:CD	1:C:429:LEU:H	2.25	0.43
1:A:274:MET:HE3	1:A:351:PHE:CD2	2.37	0.43
1:B:211:GLN:HA	1:D:427:ARG:HH21	1.83	0.43
1:C:389:GLY:C	1:C:391:HIS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:399:MET:HE2	1:C:399:MET:HB2	1.87	0.42
1:A:372:VAL:CG2	1:A:399:MET:HE1	2.49	0.42
1:D:317:ILE:H	1:D:317:ILE:HD12	1.84	0.42
1:C:379:PRO:HD3	1:C:399:MET:HE1	2.02	0.42
1:C:401:ASN:OD1	1:C:401:ASN:N	2.53	0.42
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:D:418:ARG:HA	1:D:421:MET:HE3	2.02	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%)	12	39
1	B	191/231 (83%)	175 (92%)	15 (8%)	1 (0%)	24	54
1	C	199/231 (86%)	177 (89%)	20 (10%)	2 (1%)	12	39
1	D	201/231 (87%)	179 (89%)	17 (8%)	5 (2%)	4	17
All	All	786/924 (85%)	706 (90%)	70 (9%)	10 (1%)	9	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	429	LEU
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%)	160 (99%)	2 (1%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	154/204 (76%)	151 (98%)	3 (2%)	50	79
1	C	162/204 (79%)	162 (100%)	0	100	100
1	D	162/204 (79%)	160 (99%)	2 (1%)	63	86
All	All	640/816 (78%)	633 (99%)	7 (1%)	65	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	VAL
1	A	428	GLN
1	B	238	SER
1	B	240	ASN
1	B	359	SER
1	D	241	GLU
1	D	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	277	GLN
1	A	357	GLN
1	B	282	HIS
1	C	277	GLN
1	D	237	ASN
1	D	277	GLN
1	D	401	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 [i](#)

There are no oligosaccharides 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, 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(Å ²)	Q<0.9
1	A	203/231 (87%)	0.82	25 (12%) 8 7	48, 71, 108, 140	0
1	B	199/231 (86%)	0.83	31 (15%) 5 4	48, 68, 105, 138	0
1	C	207/231 (89%)	0.79	25 (12%) 8 7	45, 74, 120, 142	0
1	D	207/231 (89%)	0.79	30 (14%) 6 4	44, 71, 119, 137	0
All	All	816/924 (88%)	0.81	111 (13%) 7 5	44, 71, 118, 142	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ASN	6.3
1	A	428	GLN	6.3
1	B	310	ASP	5.8
1	C	430	LEU	5.6
1	C	359	SER	5.0
1	C	237	ASN	4.9
1	A	303	GLU	4.6
1	B	201	LYS	4.6
1	B	241	GLU	4.5
1	B	261	ASP	4.4
1	C	303	GLU	4.3
1	D	399	MET	4.3
1	C	429	LEU	4.1
1	A	357	GLN	4.1
1	D	380	LEU	4.0
1	B	237	ASN	4.0
1	D	385	GLU	4.0
1	D	356	LEU	3.9
1	B	388	ASN	3.8
1	B	238	SER	3.7
1	C	301	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	391	HIS	3.6
1	D	357	GLN	3.5
1	A	310	ASP	3.5
1	D	384	VAL	3.5
1	B	277	GLN	3.4
1	D	300	LYS	3.4
1	A	356	LEU	3.4
1	A	302	ASP	3.4
1	D	220	HIS	3.3
1	B	392	ASP	3.2
1	B	385	GLU	3.2
1	B	386	GLU	3.2
1	C	361	ASN	3.2
1	A	429	LEU	3.2
1	B	202	HIS	3.2
1	D	299	THR	3.1
1	C	302	ASP	3.1
1	B	360	VAL	3.1
1	D	372	VAL	3.1
1	C	390	SER	3.0
1	D	310	ASP	3.0
1	C	417	LEU	3.0
1	C	360	VAL	3.0
1	D	379	PRO	3.0
1	A	220	HIS	3.0
1	B	280	ASP	3.0
1	A	272	THR	2.9
1	A	355	PHE	2.9
1	D	301	THR	2.9
1	B	219	VAL	2.9
1	B	356	LEU	2.9
1	D	331	LEU	2.9
1	A	392	ASP	2.8
1	B	359	SER	2.8
1	A	362	LYS	2.8
1	D	381	TYR	2.7
1	C	403	VAL	2.7
1	C	419	ALA	2.7
1	C	220	HIS	2.7
1	D	240	ASN	2.7
1	D	326	SER	2.7
1	C	327	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	410	PRO	2.7
1	C	388	ASN	2.7
1	A	430	LEU	2.7
1	D	397	CYS	2.6
1	B	387	GLY	2.6
1	C	358	GLU	2.6
1	A	298	LYS	2.6
1	A	242	ARG	2.5
1	B	239	HIS	2.5
1	C	400	GLY	2.5
1	C	393	PHE	2.5
1	D	272	THR	2.5
1	A	409	ALA	2.5
1	C	362	LYS	2.5
1	B	394	VAL	2.5
1	A	393	PHE	2.4
1	C	428	GLN	2.4
1	C	384	VAL	2.4
1	D	383	VAL	2.4
1	B	390	SER	2.3
1	B	206	PRO	2.3
1	A	390	SER	2.3
1	A	203	PRO	2.3
1	A	360	VAL	2.3
1	B	391	HIS	2.3
1	B	405	GLY	2.3
1	D	277	GLN	2.2
1	C	219	VAL	2.2
1	B	355	PHE	2.2
1	D	269	GLY	2.2
1	D	295	LYS	2.2
1	B	363	GLU	2.2
1	C	386	GLU	2.2
1	D	361	ASN	2.2
1	D	391	HIS	2.1
1	A	276	SER	2.1
1	A	354	ASN	2.1
1	B	429	LEU	2.1
1	D	245	PHE	2.1
1	C	357	GLN	2.1
1	D	360	VAL	2.1
1	B	311	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	428	GLN	2.0
1	D	270	LYS	2.0
1	B	204	PRO	2.0
1	A	331	LEU	2.0
1	D	408	LYS	2.0
1	D	382	VAL	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 oligosaccharides 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.