



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 10:41 AM EST

PDB ID : 5X70
Title : Crystal structure of Rice Dwarf Virus P5 in complex with a ssRNA oligomer
Authors : Nakamichi, Y.; Higashiura, A.; Nakagawa, A.
Deposited on : 2017-02-23
Resolution : 3.30 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 ⓘ symbol.

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

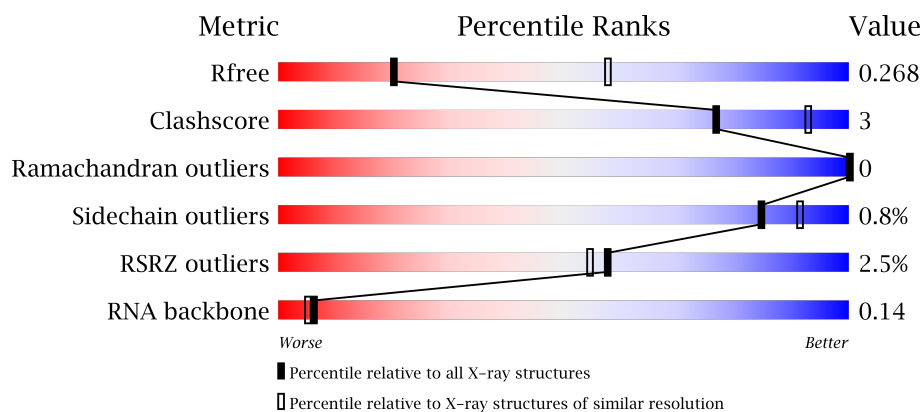
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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 $\leq 5\%$. 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	804	
1	B	804	
1	C	804	
1	D	804	

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Mol	Chain	Length	Quality of chain
2	E	6	 50% 50%
2	G	6	 17% 17% 67%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24258 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 mRNA capping enzyme P5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total	C	N	O	S	0	0	0
			6193	3990	1026	1140	37			
1	C	753	Total	C	N	O	S	0	0	0
			5968	3847	987	1097	37			
1	D	730	Total	C	N	O	S	0	0	0
			5788	3729	955	1068	36			
1	B	780	Total	C	N	O	S	0	0	0
			6200	3995	1027	1141	37			

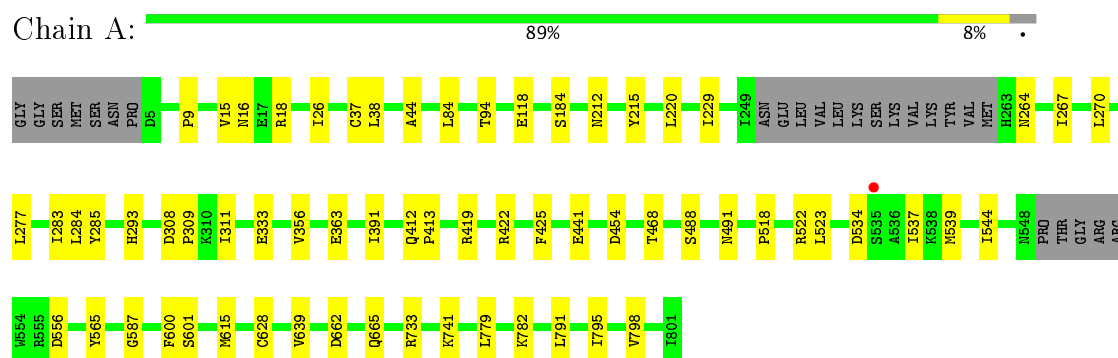
- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*GP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	P	0	0	0
			66	29	13	21	3			
2	G	2	Total	C	N	O	P	0	0	0
			43	19	8	14	2			

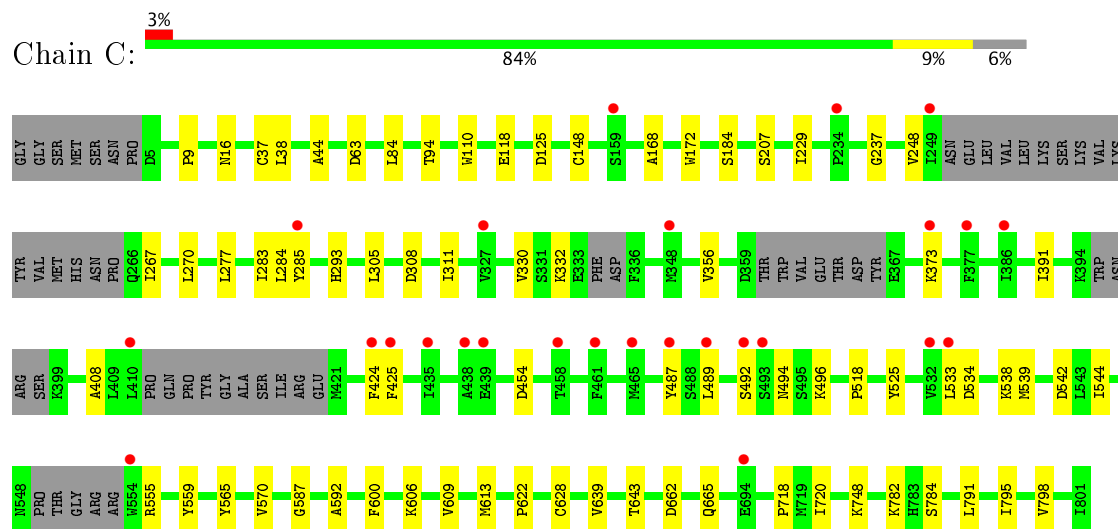
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

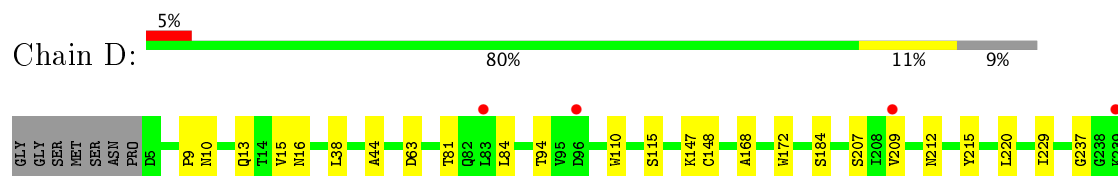
• Molecule 1: mRNA capping enzyme P5

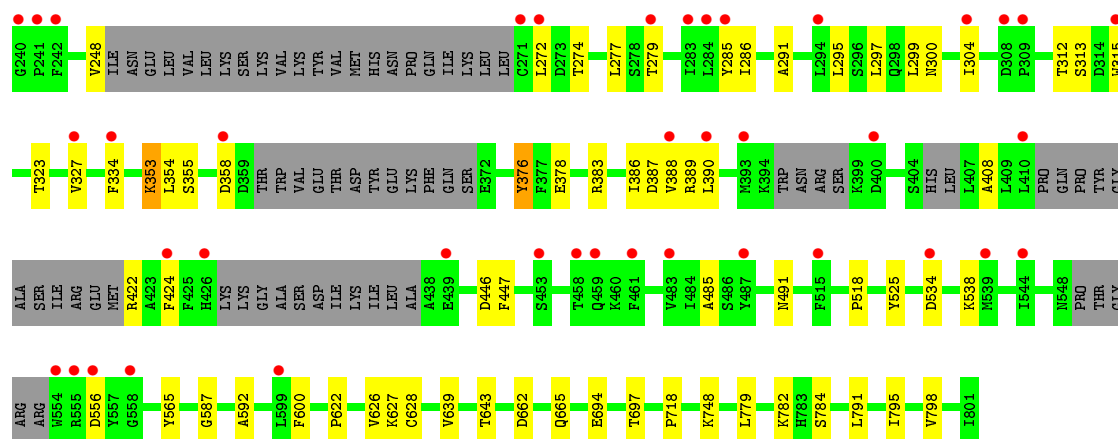


• Molecule 1: mRNA capping enzyme P5

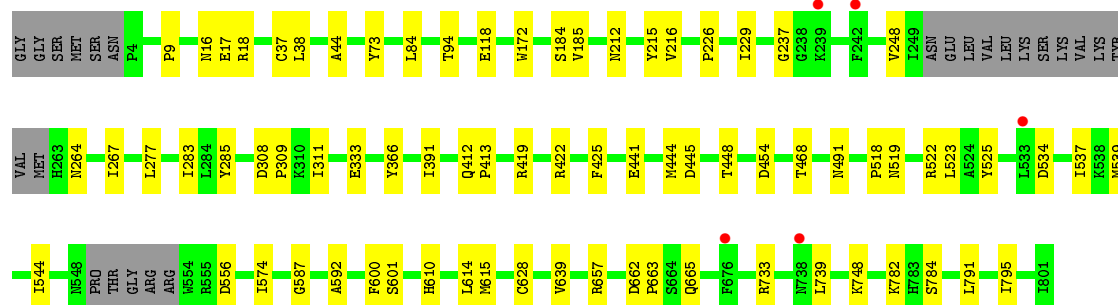
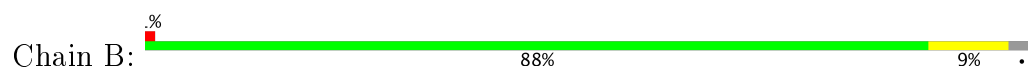


• Molecule 1: mRNA capping enzyme P5





- Molecule 1: mRNA capping enzyme P5



- Molecule 2: RNA (5'-R(P*GP*GP*CP*AP*AP*A)-3')



- Molecule 2: RNA (5'-R(P*GP*GP*CP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.75Å 80.66Å 145.73Å 104.74° 104.00° 95.29°	Depositor
Resolution (Å)	38.53 – 3.30 38.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.53-3.30) 87.6 (38.53-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.32Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.220 , 0.269 0.218 , 0.268	Depositor DCC
R_{free} test set	2667 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.400 for k,h,-h-k-l 0.013 for -k,-h,l 0.009 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24258	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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	0.24	0/6343	0.39	0/8608
1	B	0.24	0/6351	0.39	0/8619
1	C	0.24	0/6103	0.38	0/8270
1	D	0.25	0/5921	0.42	0/8028
2	E	0.15	0/73	0.68	0/112
2	G	0.44	0/47	1.02	0/71
All	All	0.24	0/24838	0.40	0/33708

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	6193	0	6185	36	0
1	B	6200	0	6193	39	0
1	C	5968	0	5988	44	0
1	D	5788	0	5773	51	0
2	E	66	0	34	0	0
2	G	43	0	23	1	0
All	All	24258	0	24196	167	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 3.

All (167) 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:D:388:VAL:O	1:D:389:ARG:HD2	1.74	0.86
1:C:391:ILE:HB	1:C:425:PHE:HB2	1.69	0.73
1:D:408:ALA:HB3	1:D:424:PHE:HB2	1.74	0.69
1:D:291:ALA:HB2	1:D:315:TRP:HE1	1.57	0.69
1:A:662:ASP:HB3	1:A:665:GLN:HG3	1.78	0.66
1:A:264:ASN:HB3	1:A:267:ILE:HB	1.79	0.64
1:A:391:ILE:HB	1:A:425:PHE:HB2	1.80	0.64
1:D:626:VAL:HG23	1:D:627:LYS:HG2	1.78	0.64
1:A:308:ASP:HB3	1:A:311:ILE:HG13	1.80	0.63
1:C:16:ASN:HA	1:C:782:LYS:HE3	1.81	0.63
1:D:291:ALA:HB2	1:D:315:TRP:NE1	2.15	0.62
1:B:308:ASP:HB3	1:B:311:ILE:HG13	1.81	0.61
1:C:489:LEU:O	1:C:494:ASN:ND2	2.24	0.61
1:D:279:THR:HG21	1:D:390:LEU:HD22	1.82	0.61
1:D:16:ASN:HA	1:D:782:LYS:HE3	1.84	0.59
1:B:413:PRO:HD2	1:B:422:ARG:HH12	1.68	0.59
1:D:286:ILE:HG23	1:D:358:ASP:HA	1.85	0.59
1:D:299:LEU:HB2	1:D:323:THR:HG23	1.86	0.58
1:B:264:ASN:HB3	1:B:267:ILE:HB	1.86	0.57
1:A:16:ASN:HA	1:A:782:LYS:HE3	1.87	0.56
1:D:378:GLU:OE1	1:D:378:GLU:N	2.39	0.56
1:B:391:ILE:HB	1:B:425:PHE:HB2	1.89	0.55
1:C:284:LEU:HB3	1:C:356:VAL:HG22	1.90	0.54
1:D:81:THR:HG22	1:D:627:LYS:HB3	1.89	0.54
1:D:662:ASP:HB3	1:D:665:GLN:HG3	1.88	0.54
1:A:9:PRO:HB3	1:A:639:VAL:HG22	1.89	0.54
1:C:662:ASP:HB3	1:C:665:GLN:HG3	1.89	0.54
1:B:662:ASP:HB3	1:B:665:GLN:HG3	1.90	0.54
1:C:492:SER:HB2	1:C:555:ARG:HB2	1.91	0.53
1:B:309:PRO:HG3	1:B:333:GLU:HG2	1.91	0.53
1:B:657:ARG:HE	1:B:663:PRO:HG3	1.73	0.53
1:B:16:ASN:HA	1:B:782:LYS:HE3	1.90	0.53
1:D:297:LEU:HB3	1:D:299:LEU:HD13	1.91	0.53
1:B:444:MET:O	1:B:448:THR:OG1	2.20	0.52
1:A:419:ARG:HH21	1:A:441:GLU:HG3	1.74	0.52
1:B:522:ARG:NH2	1:B:601:SER:OG	2.43	0.52
1:C:533:LEU:HD23	1:C:533:LEU:H	1.74	0.52
1:A:309:PRO:HG3	1:A:333:GLU:HG2	1.92	0.52
1:D:272:LEU:HD22	1:D:422:ARG:HE	1.74	0.52
1:C:539:MET:HG3	1:C:544:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:PRO:HD2	1:A:422:ARG:HH12	1.75	0.51
1:A:488:SER:O	1:A:491:ASN:ND2	2.38	0.51
1:A:184:SER:OG	1:A:587:GLY:HA3	2.11	0.51
1:B:419:ARG:HH21	1:B:441:GLU:HG2	1.76	0.50
1:B:9:PRO:HB3	1:B:639:VAL:HG22	1.94	0.50
1:C:570:VAL:HG13	1:C:720:ILE:HG12	1.92	0.50
1:A:539:MET:HG3	1:A:544:ILE:HG12	1.94	0.50
1:C:308:ASP:HB3	1:C:311:ILE:HG13	1.94	0.50
1:D:286:ILE:HD12	1:D:334:PHE:CG	2.47	0.49
1:D:622:PRO:HB3	1:D:718:PRO:HG2	1.93	0.49
1:A:84:LEU:HG	1:A:628:CYS:HB2	1.94	0.49
1:B:184:SER:OG	1:B:587:GLY:HA3	2.12	0.49
1:C:184:SER:OG	1:C:587:GLY:HA3	2.12	0.49
1:B:539:MET:HG3	1:B:544:ILE:HG12	1.94	0.49
1:D:209:VAL:HB	1:D:485:ALA:HA	1.95	0.48
1:B:615:MET:HE3	1:B:733:ARG:HB2	1.95	0.48
1:A:284:LEU:HB3	1:A:356:VAL:HG12	1.95	0.48
1:D:694:GLU:O	1:D:697:THR:OG1	2.29	0.48
1:D:791:LEU:O	1:D:795:ILE:HG12	2.13	0.48
1:C:9:PRO:HB3	1:C:639:VAL:HG22	1.95	0.48
1:A:356:VAL:HG22	1:A:391:ILE:HG12	1.96	0.47
1:D:184:SER:OG	1:D:587:GLY:HA3	2.14	0.47
1:A:615:MET:HE3	1:A:733:ARG:HB2	1.97	0.47
1:A:491:ASN:HA	1:A:556:ASP:HA	1.95	0.47
1:D:274:THR:HA	1:D:277:LEU:HD12	1.96	0.47
1:D:525:TYR:CD1	1:D:784:SER:HB2	2.50	0.47
1:C:622:PRO:HB3	1:C:718:PRO:HG2	1.96	0.47
1:D:353:LYS:HA	1:D:387:ASP:HB3	1.97	0.47
1:C:267:ILE:HD12	1:C:270:LEU:HB2	1.97	0.47
1:C:791:LEU:O	1:C:795:ILE:HG12	2.14	0.47
1:D:565:TYR:CZ	1:D:798:VAL:HG22	2.50	0.46
1:C:330:VAL:HG12	1:C:332:LYS:H	1.80	0.46
1:D:9:PRO:HB3	1:D:639:VAL:HG22	1.96	0.46
1:C:270:LEU:HG	1:C:293:HIS:HB2	1.98	0.46
1:D:110:TRP:CD1	1:D:148:CYS:HA	2.51	0.46
1:A:522:ARG:NH2	1:A:601:SER:OG	2.49	0.46
1:C:542:ASP:N	1:C:542:ASP:OD1	2.49	0.46
1:C:408:ALA:HB3	1:C:424:PHE:HB2	1.98	0.46
1:A:518:PRO:HG3	1:A:600:PHE:CE2	2.50	0.45
1:C:565:TYR:CD1	1:C:720:ILE:HD11	2.51	0.45
1:B:84:LEU:HG	1:B:628:CYS:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ASN:HA	1:B:556:ASP:HA	1.98	0.45
1:C:277:LEU:HD23	1:C:283:ILE:HG13	1.97	0.45
1:C:110:TRP:CD1	1:C:148:CYS:HA	2.52	0.45
1:C:565:TYR:CZ	1:C:798:VAL:HG22	2.52	0.45
1:B:38:LEU:HD21	1:B:44:ALA:HB2	1.98	0.45
1:B:791:LEU:O	1:B:795:ILE:HG12	2.17	0.45
1:C:38:LEU:O	1:C:94:THR:HA	2.17	0.45
1:D:378:GLU:O	1:D:378:GLU:HG2	2.16	0.45
1:B:212:ASN:HB3	1:B:215:TYR:HD2	1.83	0.44
1:B:518:PRO:HG3	1:B:600:PHE:CE2	2.52	0.44
1:C:525:TYR:CD1	1:C:784:SER:HB2	2.52	0.44
1:C:748:LYS:HE2	1:C:748:LYS:HB3	1.83	0.44
1:D:491:ASN:HA	1:D:556:ASP:HA	1.99	0.44
1:C:496:LYS:HA	1:C:559:TYR:OH	2.17	0.44
1:D:304:ILE:HB	1:D:327:VAL:HG13	1.99	0.44
1:A:38:LEU:HD21	1:A:44:ALA:HB2	1.99	0.44
1:D:38:LEU:HD21	1:D:44:ALA:HB2	1.99	0.44
1:A:270:LEU:HG	1:A:293:HIS:HB2	2.00	0.44
1:C:38:LEU:HD21	1:C:44:ALA:HB2	2.00	0.44
1:D:518:PRO:HG3	1:D:600:PHE:CE2	2.53	0.44
1:D:748:LYS:HE2	1:D:748:LYS:HB3	1.81	0.44
1:A:26:ILE:HG22	1:A:84:LEU:HD22	2.00	0.43
1:C:518:PRO:HG3	1:C:600:PHE:CE2	2.53	0.43
1:C:168:ALA:HB1	1:D:643:THR:HG23	1.99	0.43
1:C:207:SER:HB3	1:C:229:ILE:HD12	2.00	0.43
1:B:37:CYS:HB2	1:B:118:GLU:HA	2.01	0.43
1:D:312:THR:OG1	1:D:313:SER:N	2.51	0.43
1:B:216:VAL:HA	1:B:226:PRO:HG3	2.00	0.43
1:C:565:TYR:CE1	1:C:606:LYS:HD2	2.54	0.43
1:D:84:LEU:HG	1:D:628:CYS:HB2	2.01	0.43
1:B:73:TYR:OH	2:G:3:C:OP1	2.28	0.43
1:A:791:LEU:O	1:A:795:ILE:HG12	2.18	0.43
1:D:207:SER:HB3	1:D:229:ILE:HD12	2.01	0.43
1:C:172:TRP:HZ2	1:C:592:ALA:HB2	1.84	0.42
1:D:38:LEU:O	1:D:94:THR:HA	2.18	0.42
1:A:277:LEU:HD23	1:A:283:ILE:HG13	2.01	0.42
1:A:412:GLN:HG2	1:A:422:ARG:HG3	2.00	0.42
1:B:412:GLN:HG2	1:B:422:ARG:HG3	2.01	0.42
1:C:284:LEU:HD13	1:C:305:LEU:HD23	2.01	0.42
1:D:237:GLY:HA3	1:D:248:VAL:HG23	2.01	0.42
1:D:63:ASP:HA	1:D:94:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:ASN:HB3	1:D:215:TYR:HD2	1.84	0.42
1:C:237:GLY:HA3	1:C:248:VAL:HG23	2.01	0.42
1:D:172:TRP:HZ2	1:D:592:ALA:HB2	1.83	0.42
1:C:570:VAL:HB	1:C:609:VAL:HG21	2.02	0.42
1:D:295:LEU:HD12	1:D:295:LEU:HA	1.81	0.42
1:A:523:LEU:HD21	1:A:537:ILE:HG21	2.00	0.42
1:A:15:VAL:HG11	1:A:779:LEU:HA	2.02	0.42
1:B:523:LEU:HD21	1:B:537:ILE:HG21	2.02	0.42
1:D:15:VAL:HG11	1:D:779:LEU:HA	2.00	0.42
1:A:37:CYS:HB2	1:A:118:GLU:HA	2.01	0.42
1:A:212:ASN:HB3	1:A:215:TYR:HD2	1.84	0.42
1:B:172:TRP:HZ2	1:B:592:ALA:HB2	1.85	0.42
1:A:18:ARG:HD3	1:B:18:ARG:NH2	2.35	0.42
1:B:277:LEU:HD23	1:B:283:ILE:HG13	2.01	0.41
1:A:38:LEU:O	1:A:94:THR:HA	2.20	0.41
1:B:519:ASN:OD1	1:B:522:ARG:HB2	2.20	0.41
1:B:17:GLU:OE2	1:B:782:LYS:NZ	2.44	0.41
1:C:643:THR:HG23	1:D:168:ALA:HB1	2.02	0.41
1:C:84:LEU:HG	1:C:628:CYS:HB2	2.03	0.41
1:B:525:TYR:CD1	1:B:784:SER:HB2	2.55	0.41
1:C:538:LYS:HD2	1:C:538:LYS:HA	1.80	0.41
1:D:115:SER:OG	1:D:147:LYS:HG3	2.21	0.41
1:A:267:ILE:HD12	1:A:270:LEU:HB2	2.02	0.41
1:C:356:VAL:HB	1:C:391:ILE:HD13	2.02	0.41
1:D:386:ILE:HG23	1:D:388:VAL:HG23	2.02	0.41
1:B:229:ILE:HA	1:B:468:THR:O	2.20	0.41
1:B:185:VAL:HG11	1:B:574:ILE:HG23	2.03	0.41
1:D:10:ASN:HD21	1:D:13:GLN:HG2	1.85	0.41
1:C:609:VAL:HA	1:C:613:MET:HB2	2.03	0.41
1:C:63:ASP:HA	1:C:94:THR:OG1	2.20	0.41
1:D:538:LYS:HA	1:D:538:LYS:HD2	1.81	0.41
1:A:220:LEU:HD13	1:A:220:LEU:HA	1.96	0.41
1:A:741:LYS:HG2	1:A:741:LYS:H	1.63	0.41
1:B:610:HIS:HA	1:B:614:LEU:HG	2.03	0.41
1:C:373:LYS:HE3	1:C:373:LYS:HB2	1.86	0.41
1:A:565:TYR:CZ	1:A:798:VAL:HG22	2.56	0.41
1:B:419:ARG:HH22	1:B:445:ASP:CG	2.23	0.40
1:A:229:ILE:HA	1:A:468:THR:O	2.22	0.40
1:B:237:GLY:HA3	1:B:248:VAL:HG23	2.03	0.40
1:B:739:LEU:HD23	1:B:739:LEU:HA	1.89	0.40
1:C:37:CYS:HB2	1:C:118:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:O	1:B:94:THR:HA	2.21	0.40
1:D:220:LEU:HA	1:D:220:LEU:HD13	1.89	0.40
1:D:354:LEU:HD13	1:D:355:SER:N	2.37	0.40
1:D:376:TYR:O	1:D:376:TYR:HD1	2.05	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	773/804 (96%)	743 (96%)	30 (4%)	0	100	100
1	B	774/804 (96%)	742 (96%)	32 (4%)	0	100	100
1	C	739/804 (92%)	704 (95%)	35 (5%)	0	100	100
1	D	714/804 (89%)	673 (94%)	41 (6%)	0	100	100
All	All	3000/3216 (93%)	2862 (95%)	138 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	689/711 (97%)	685 (99%)	4 (1%)	89	93
1	B	690/711 (97%)	685 (99%)	5 (1%)	87	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	665/711 (94%)	660 (99%)	5 (1%)	85	91
1	D	645/711 (91%)	637 (99%)	8 (1%)	75	87
All	All	2689/2844 (94%)	2667 (99%)	22 (1%)	85	91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	TYR
1	A	363	GLU
1	A	454	ASP
1	A	534	ASP
1	C	125	ASP
1	C	285	TYR
1	C	454	ASP
1	C	487	TYR
1	C	534	ASP
1	D	285	TYR
1	D	300	ASN
1	D	353	LYS
1	D	376	TYR
1	D	383	ARG
1	D	446	ASP
1	D	447	PHE
1	D	534	ASP
1	B	285	TYR
1	B	366	TYR
1	B	454	ASP
1	B	534	ASP
1	B	748	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	374	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	3/6 (50%)	2 (66%)	1 (33%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	1/6 (16%)	0	0
All	All	4/12 (33%)	2 (50%)	1 (25%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	G
2	E	3	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	1	G

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, 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	779/804 (96%)	-0.11	1 (0%) 95 96	42, 66, 97, 115	0
1	B	780/804 (97%)	-0.09	5 (0%) 89 88	43, 66, 98, 118	0
1	C	753/804 (93%)	0.18	26 (3%) 44 41	47, 81, 136, 160	0
1	D	730/804 (90%)	0.27	44 (6%) 23 21	46, 80, 133, 160	0
2	E	3/6 (50%)	0.85	0 100 100	90, 90, 102, 120	0
2	G	2/6 (33%)	0.21	0 100 100	89, 89, 89, 101	0
All	All	3047/3228 (94%)	0.06	76 (2%) 58 54	42, 71, 126, 160	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	THR	5.7
1	D	410	LEU	5.6
1	D	390	LEU	5.0
1	C	234	PRO	4.9
1	D	304	ILE	4.8
1	D	424	PHE	4.6
1	D	461	PHE	4.5
1	D	294	LEU	4.3
1	C	377	PHE	4.1
1	C	465	MET	4.1
1	C	435	ILE	4.1
1	C	327	VAL	3.8
1	D	334	PHE	3.7
1	D	327	VAL	3.7
1	C	532	VAL	3.5
1	D	279	THR	3.5
1	D	283	ILE	3.5
1	C	439	GLU	3.3
1	D	285	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	453	SER	3.2
1	C	533	LEU	3.2
1	D	483	VAL	3.2
1	D	555	ARG	3.1
1	D	393	MET	3.0
1	D	271	CYS	2.9
1	B	738	ASN	2.9
1	D	544	ILE	2.9
1	D	554	TRP	2.9
1	D	240	GLY	2.8
1	C	458	THR	2.8
1	C	410	LEU	2.8
1	D	272	LEU	2.7
1	D	388	VAL	2.7
1	D	309	PRO	2.7
1	D	556	ASP	2.7
1	C	492	SER	2.7
1	D	439	GLU	2.6
1	C	461	PHE	2.6
1	D	308	ASP	2.6
1	D	459	GLN	2.5
1	B	533	LEU	2.5
1	C	425	PHE	2.5
1	D	487	TYR	2.5
1	C	285	TYR	2.4
1	D	315	TRP	2.4
1	D	558	GLY	2.4
1	C	424	PHE	2.4
1	D	242	PHE	2.4
1	D	539	MET	2.4
1	C	554	TRP	2.4
1	D	358	ASP	2.4
1	C	438	ALA	2.4
1	D	241	PRO	2.4
1	D	426	HIS	2.3
1	C	386	ILE	2.3
1	D	239	LYS	2.3
1	D	400	ASP	2.3
1	C	373	LYS	2.3
1	C	487	TYR	2.2
1	D	284	LEU	2.2
1	C	348	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	489	LEU	2.2
1	B	242	PHE	2.2
1	C	249	ILE	2.2
1	A	535	SER	2.1
1	D	534	ASP	2.1
1	D	209	VAL	2.1
1	D	83	LEU	2.1
1	D	515	PHE	2.1
1	C	493	SER	2.1
1	C	694	GLU	2.1
1	B	676	PHE	2.0
1	C	159	SER	2.0
1	D	96	ASP	2.0
1	B	239	LYS	2.0
1	D	599	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 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.