W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2017 – 04:13 PM EST

PDB ID	:	5WTY
Title	:	Structure of Nop9 RNA complex
Authors	:	Ye, K.; Wang, B.
Deposited on	:	2016-12-15
Resolution	:	2.79 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
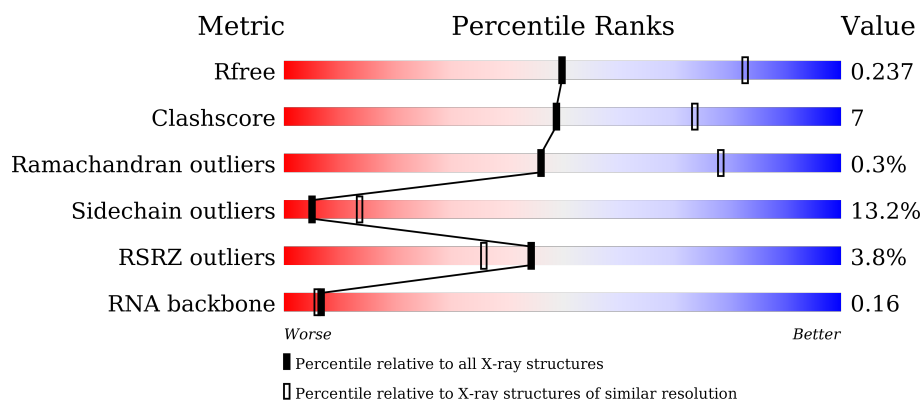with specific help available everywhere you see the ⓘ symbol.

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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
Rfree		0.237
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		13.2%
RSRZ outliers		3.8%
RNA backbone		0.16

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))
R$_{free}$	91344	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)
RNA backbone	2183	1015 (3.16-2.40)

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 <=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	587	3% / 67% / 23% / • / 7%
1	B	587	3% / 69% / 21% / • / 7%
2	C	18	11% / 28% / 22% / 6% / 6% / 39%
2	D	18	22% / 11% / 44% / 6% / 39%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9520 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 Nucleolar protein 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	547	Total 4477	C 2877	N 748	O 833	S 19	0	0	0
1	A	544	Total 4457	C 2865	N 745	O 828	S 19	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	48	GLY	-	expression tag	UNP P47077
B	49	PRO	-	expression tag	UNP P47077
B	50	GLU	-	expression tag	UNP P47077
B	51	ALA	-	expression tag	UNP P47077
B	52	SER	-	expression tag	UNP P47077
A	48	GLY	-	expression tag	UNP P47077
A	49	PRO	-	expression tag	UNP P47077
A	50	GLU	-	expression tag	UNP P47077
A	51	ALA	-	expression tag	UNP P47077
A	52	SER	-	expression tag	UNP P47077

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total 241	C 107	N 47	O 76	P 11	0	0	0
2	D	11	Total 241	C 107	N 47	O 76	P 11	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	43	Total 43	O 43	0	0
3	A	55	Total 55	O 55	0	0
3	C	4	Total 4	O 4	0	0
3	D	2	Total 2	O 2	0	0

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 errors 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: Nucleolar protein 9
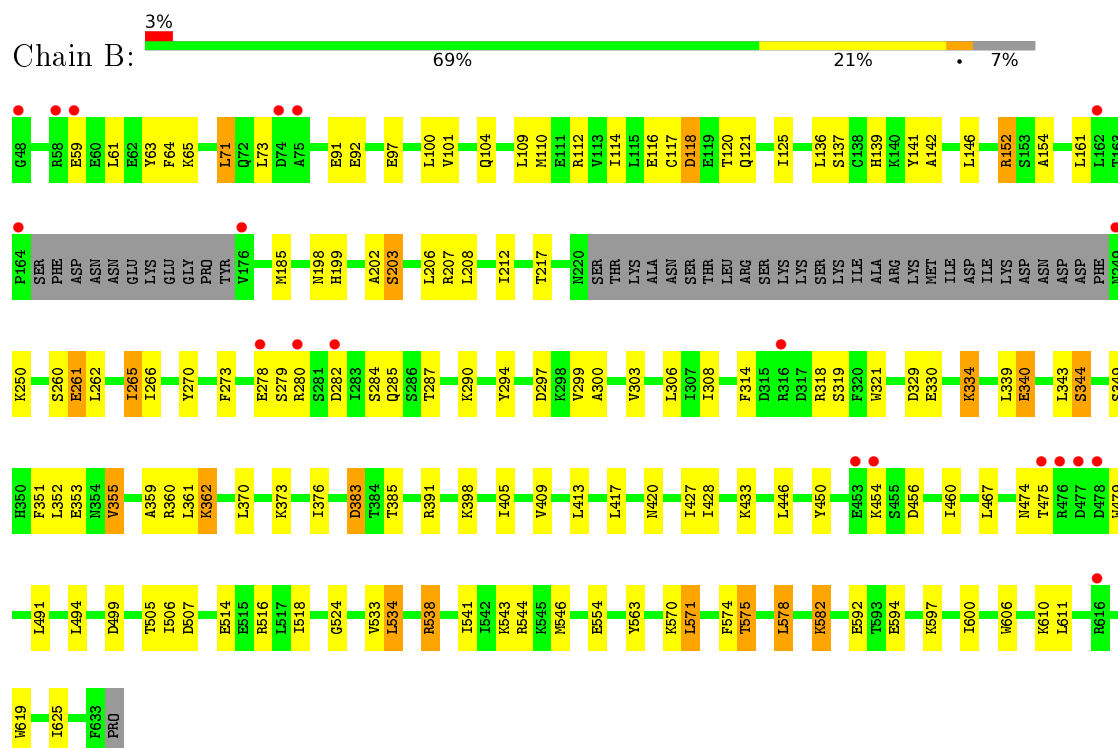
- Molecule 1: Nucleolar protein 9
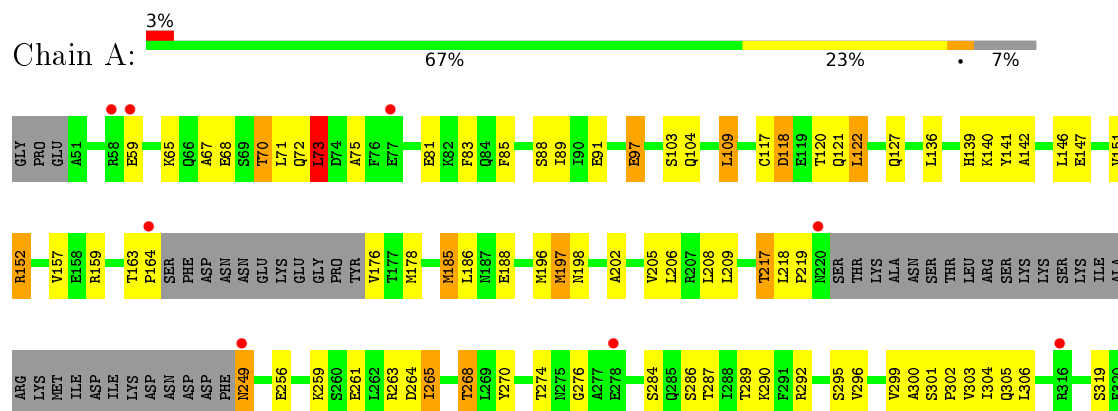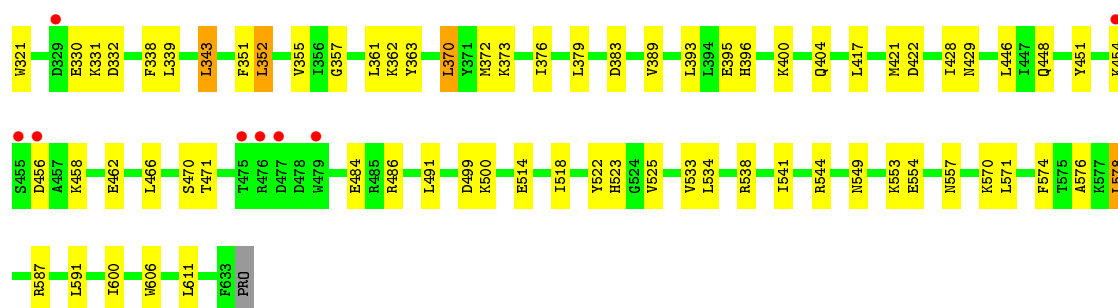
● Molecule 2: RNA (5'-R(*AP*AP*AP*GP*GP*AP*AP*UP*UP*GP*AP*CP*GP*GP*AP*AP*GP*G)-3')

● Molecule 2: RNA (5'-R(*AP*AP*AP*GP*GP*AP*AP*UP*UP*GP*AP*CP*GP*GP*AP*AP*GP*G)-3')
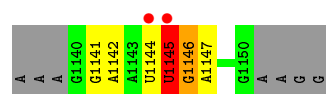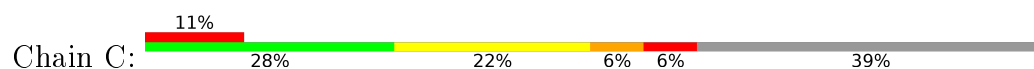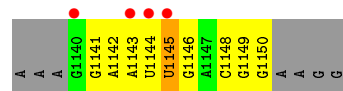
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.50Å 102.74Å 114.71Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	19.96 – 2.79 19.96 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.96-2.79) 98.0 (19.96-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.83 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.176 , 0.237 0.176 , 0.237	Depositor DCC
R_{free} test set	1975 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	41.2	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	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	0.93	EDS
Total number of atoms	9520	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 ⓘ

5.1 Standard geometry ⓘ

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	0/4538	0.62	1/6117 (0.0%)
1	B	0.45	0/4559	0.58	0/6146
2	C	0.63	0/270	1.24	1/420 (0.2%)
2	D	0.60	0/270	1.19	1/420 (0.2%)
All	All	0.47	0/9637	0.65	3/13103 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	LEU	CA-CB-CG	6.25	129.67	115.30
2	D	1145	U	C2-N1-C1'	5.64	124.47	117.70
2	C	1145	U	N3-C2-O2	-5.03	118.68	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4457	0	4533	68	0
1	B	4477	0	4549	64	0
2	C	241	0	120	2	0
2	D	241	0	120	1	0
3	A	55	0	0	1	0
3	B	43	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	0	1	0
3	D	2	0	0	0	0
All	All	9520	0	9322	135	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 7.

All (135) 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:73:LEU:HD13	1:A:75:ALA:H	1.35	0.88
1:B:499:ASP:OD1	1:B:538:ARG:NH1	2.13	0.81
1:B:362:LYS:HD2	1:B:362:LYS:H	1.53	0.73
1:B:71:LEU:HD12	1:B:112:ARG:HD3	1.71	0.72
1:B:114:ILE:HD11	1:B:125:ILE:HG21	1.72	0.71
1:A:321:TRP:HZ3	1:A:355:VAL:HG13	1.57	0.69
1:A:499:ASP:OD1	1:A:538:ARG:NH1	2.25	0.68
1:B:198:ASN:HD21	1:B:294:TYR:HE2	1.41	0.67
1:B:575:THR:HG22	1:B:582:LYS:HZ1	1.60	0.67
1:A:331:LYS:HG2	1:A:370:LEU:HG	1.77	0.67
1:B:541:ILE:HD11	1:B:578:LEU:HD13	1.75	0.67
2:C:1145:U:O2'	2:C:1146:G:OP1	2.12	0.66
1:A:600:ILE:H	1:A:600:ILE:HD12	1.61	0.66
1:B:321:TRP:HZ3	1:B:355:VAL:HG13	1.62	0.65
1:A:264:ASP:O	1:A:268:THR:HG23	1.96	0.64
1:B:104:GLN:HB3	1:B:141:TYR:CZ	2.34	0.62
1:A:139:HIS:HB3	1:A:142:ALA:HB3	1.82	0.61
1:B:544:ARG:NH2	3:B:703:HOH:O	2.33	0.61
1:B:376:ILE:HG12	1:B:405:ILE:HG12	1.81	0.60
1:B:571:LEU:O	1:B:575:THR:HB	2.01	0.60
1:B:383:ASP:HB3	1:B:420:ASN:HB2	1.82	0.59
1:A:373:LYS:NZ	1:A:404:GLN:OE1	2.35	0.59
1:A:198:ASN:HB3	1:A:300:ALA:HB2	1.85	0.57
1:A:185:MET:HE1	1:A:186:LEU:HD23	1.87	0.57
1:A:217:THR:HG1	1:A:249:ASN:N	2.02	0.56
1:A:544:ARG:HG2	1:A:574:PHE:CZ	2.40	0.56
1:B:117:CYS:O	1:B:152:ARG:NH2	2.36	0.56
1:A:541:ILE:HD11	1:A:578:LEU:HD13	1.87	0.56
1:B:383:ASP:N	1:B:383:ASP:OD1	2.37	0.56
1:B:600:ILE:HD12	1:B:600:ILE:H	1.71	0.56
1:A:163:THR:N	1:A:164:PRO:HD3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:GLY:HA2	1:B:563:TYR:CZ	2.42	0.55
1:A:117:CYS:O	1:A:152:ARG:NH2	2.39	0.54
1:B:270:TYR:CE1	1:B:319:SER:HB3	2.42	0.54
1:B:518:ILE:HD12	1:B:554:GLU:HG3	1.90	0.54
1:B:285:GLN:HG2	1:B:334:LYS:NZ	2.23	0.54
1:A:122:LEU:HD11	1:A:152:ARG:HB3	1.90	0.54
1:A:261:GLU:O	1:A:265:ILE:HG23	2.08	0.54
1:B:446:LEU:HD13	1:B:494:LEU:HD11	1.91	0.53
1:A:176:VAL:N	3:A:701:HOH:O	2.41	0.53
1:B:139:HIS:HB3	1:B:142:ALA:HB3	1.89	0.53
2:D:1148:C:O2'	2:D:1149:G:H5'	2.08	0.53
1:B:261:GLU:O	1:B:265:ILE:HG23	2.09	0.52
1:A:256:GLU:HA	1:A:259:LYS:HD2	1.92	0.52
1:A:352:LEU:HD13	1:A:389:VAL:HG11	1.92	0.52
1:A:471:THR:HG23	1:A:484:GLU:OE2	2.10	0.52
1:A:83:PHE:CE1	1:A:118:ASP:HB3	2.45	0.51
1:B:582:LYS:HD3	1:B:625:ILE:HG12	1.92	0.51
1:B:198:ASN:ND2	1:B:294:TYR:HE2	2.08	0.51
1:B:340:GLU:O	1:B:344:SER:OG	2.29	0.51
1:B:409:VAL:HG12	1:B:427:ILE:HD11	1.93	0.51
1:A:299:VAL:O	1:A:302:PRO:HD2	2.11	0.51
1:B:385:THR:OG1	1:B:385:THR:O	2.25	0.50
2:C:1145:U:O2'	2:C:1146:G:H5"	2.11	0.50
1:B:199:HIS:O	1:B:203:SER:HB3	2.11	0.50
1:B:154:ALA:HB2	1:B:212:ILE:HD13	1.94	0.50
1:A:357:GLY:HA2	1:A:396:HIS:CE1	2.47	0.50
1:A:351:PHE:O	1:A:355:VAL:HB	2.13	0.49
1:B:362:LYS:NZ	3:B:704:HOH:O	2.42	0.49
1:B:575:THR:HG22	1:B:582:LYS:NZ	2.26	0.49
1:A:295:SER:HA	1:A:304:ILE:HD12	1.94	0.49
1:B:351:PHE:O	1:B:355:VAL:HB	2.12	0.49
1:B:450:TYR:HB3	1:B:460:ILE:HG13	1.94	0.49
1:B:606:TRP:CE3	1:B:611:LEU:HD12	2.48	0.48
1:A:372:MET:HE3	1:A:393:LEU:HD11	1.95	0.48
1:B:61:LEU:O	1:B:65:LYS:HB2	2.14	0.48
1:A:372:MET:CE	1:A:393:LEU:HD11	2.44	0.48
1:A:118:ASP:H	1:A:121:GLN:HE21	1.61	0.48
1:B:409:VAL:CG1	1:B:427:ILE:HD11	2.44	0.47
1:B:506:ILE:HG21	1:B:543:LYS:HD3	1.95	0.47
1:A:249:ASN:N	1:A:249:ASN:HD22	2.13	0.47
1:A:549:ASN:O	1:A:553:LYS:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:HG21	1:B:355:VAL:HG22	1.97	0.47
1:A:196:MET:HG2	1:A:202:ALA:HB1	1.96	0.47
1:A:301:SER:O	1:A:305:GLN:HG3	2.15	0.47
1:A:218:LEU:HB3	1:A:219:PRO:HD2	1.97	0.47
1:B:285:GLN:HG2	1:B:334:LYS:HZ2	1.80	0.47
1:A:68:GLU:HB2	1:A:109:LEU:HG	1.96	0.46
1:A:343:LEU:HG	1:A:379:LEU:HD22	1.97	0.46
1:B:199:HIS:HB3	1:B:202:ALA:HB3	1.97	0.46
1:A:514:GLU:O	1:A:518:ILE:HG12	2.16	0.46
1:B:118:ASP:HB3	1:B:121:GLN:H	1.80	0.46
1:A:606:TRP:CE3	1:A:611:LEU:HD12	2.51	0.46
1:A:104:GLN:HG3	1:A:141:TYR:CZ	2.51	0.46
1:A:522:TYR:OH	1:A:557:ASN:HB3	2.16	0.46
1:B:428:ILE:HD11	1:B:446:LEU:HD11	1.97	0.46
1:B:104:GLN:HB3	1:B:141:TYR:CE1	2.51	0.46
1:A:140:LYS:NZ	3:C:1201:HOH:O	2.49	0.45
1:A:523:HIS:HE1	1:A:525:VAL:HG22	1.82	0.45
1:B:207:ARG:HG3	1:B:303:VAL:HG22	1.98	0.45
1:B:297:ASP:HB3	1:B:300:ALA:HB3	1.99	0.45
1:B:544:ARG:HG2	1:B:574:PHE:CZ	2.51	0.45
1:B:507:ASP:OD1	1:B:543:LYS:HE3	2.17	0.45
1:A:270:TYR:CZ	1:A:274:THR:HG21	2.52	0.45
1:A:523:HIS:CE1	1:A:525:VAL:HG22	2.52	0.44
1:A:97:GLU:HG2	1:A:97:GLU:H	1.23	0.44
1:A:451:TYR:CE1	1:A:458:LYS:HB3	2.52	0.44
1:A:67:ALA:HA	1:A:70:THR:HG23	1.99	0.44
1:A:362:LYS:HE3	1:A:363:TYR:CE1	2.52	0.44
1:A:422:ASP:OD2	1:A:486:ARG:HD3	2.16	0.44
1:B:321:TRP:CZ3	1:B:355:VAL:HG13	2.48	0.44
1:A:383:ASP:N	1:A:383:ASP:OD1	2.40	0.44
1:A:470:SER:HB2	1:A:484:GLU:OE2	2.17	0.44
1:A:157:VAL:HG23	1:A:178:MET:HG3	2.00	0.44
1:A:321:TRP:CZ3	1:A:355:VAL:HG13	2.46	0.44
1:A:197:MET:HG2	1:A:303:VAL:HG11	2.00	0.43
1:B:118:ASP:HB2	1:B:121:GLN:NE2	2.33	0.43
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.85	0.43
1:B:262:LEU:O	1:B:266:ILE:HG12	2.18	0.43
1:A:428:ILE:HD11	1:A:446:LEU:HD11	2.00	0.43
1:A:85:PHE:O	1:A:89:ILE:HG13	2.18	0.43
1:B:284:SER:OG	1:B:287:THR:HG23	2.19	0.43
1:A:514:GLU:OE1	1:A:553:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:TRP:CD1	1:B:479:TRP:N	2.86	0.43
1:B:64:PHE:CD2	1:B:100:LEU:HD21	2.54	0.42
1:A:362:LYS:HB3	1:A:362:LYS:HE2	1.79	0.42
1:A:458:LYS:HE2	1:A:458:LYS:HB2	1.69	0.42
1:B:597:LYS:HE3	1:B:606:TRP:CE2	2.55	0.42
1:A:205:VAL:O	1:A:209:LEU:HG	2.21	0.41
1:A:446:LEU:HD23	1:A:446:LEU:HA	1.87	0.41
1:B:290:LYS:HE3	1:B:290:LYS:HB2	1.65	0.41
1:B:321:TRP:CZ3	1:B:359:ALA:HB2	2.54	0.41
1:A:544:ARG:NH1	1:A:576:ALA:O	2.50	0.41
1:A:284:SER:OG	1:A:287:THR:HG23	2.20	0.41
1:A:292:ARG:HD3	1:A:338:PHE:CG	2.55	0.41
1:A:65:LYS:HB3	1:A:65:LYS:HE2	1.69	0.41
1:A:147:GLU:O	1:A:151:VAL:HG23	2.19	0.41
1:B:533:VAL:HG12	1:B:534:LEU:HD13	2.02	0.41
1:B:63:TYR:CZ	1:B:92:GLU:HG3	2.56	0.41
1:B:279:SER:O	1:B:282:ASP:N	2.47	0.41
1:A:186:LEU:HD13	1:A:261:GLU:HG2	2.02	0.41
1:B:110:MET:O	1:B:114:ILE:HG12	2.21	0.40
1:B:494:LEU:HD12	1:B:494:LEU:HA	1.91	0.40
1:B:413:LEU:HD13	1:B:427:ILE:HD12	2.04	0.40
1:A:518:ILE:HD12	1:A:554:GLU:HG3	2.04	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	538/587 (92%)	519 (96%)	18 (3%)	1 (0%)	52	84
1	B	541/587 (92%)	514 (95%)	25 (5%)	2 (0%)	39	73
All	All	1079/1174 (92%)	1033 (96%)	43 (4%)	3 (0%)	46	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	278	GLU
1	A	276	GLY
1	B	280	ARG

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	499/538 (93%)	437 (88%)	62 (12%)	6	16
1	B	501/538 (93%)	431 (86%)	70 (14%)	4	12
All	All	1000/1076 (93%)	868 (87%)	132 (13%)	5	13

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	GLU
1	B	71	LEU
1	B	91	GLU
1	B	97	GLU
1	B	101	VAL
1	B	109	LEU
1	B	116	GLU
1	B	118	ASP
1	B	120	THR
1	B	136	LEU
1	B	137	SER
1	B	146	LEU
1	B	152	ARG
1	B	161	LEU
1	B	185	MET
1	B	203	SER
1	B	206	LEU
1	B	208	LEU
1	B	217	THR
1	B	250	LYS

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Mol	Chain	Res	Type
1	B	260	SER
1	B	261	GLU
1	B	265	ILE
1	B	273	PHE
1	B	299	VAL
1	B	306	LEU
1	B	314	PHE
1	B	318	ARG
1	B	329	ASP
1	B	330	GLU
1	B	334	LYS
1	B	339	LEU
1	B	340	GLU
1	B	343	LEU
1	B	344	SER
1	B	349	SER
1	B	352	LEU
1	B	353	GLU
1	B	355	VAL
1	B	360	ARG
1	B	361	LEU
1	B	362	LYS
1	B	370	LEU
1	B	373	LYS
1	B	383	ASP
1	B	391	ARG
1	B	398	LYS
1	B	417	LEU
1	B	433	LYS
1	B	454	LYS
1	B	456	ASP
1	B	467	LEU
1	B	474	ASN
1	B	475	THR
1	B	491	LEU
1	B	505	THR
1	B	514	GLU
1	B	516	ARG
1	B	534	LEU
1	B	538	ARG
1	B	546	MET
1	B	570	LYS

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Mol	Chain	Res	Type
1	B	571	LEU
1	B	575	THR
1	B	578	LEU
1	B	582	LYS
1	B	592	GLU
1	B	594	GLU
1	B	610	LYS
1	B	619	TRP
1	A	59	GLU
1	A	70	THR
1	A	71	LEU
1	A	72	GLN
1	A	73	LEU
1	A	81	GLU
1	A	88	SER
1	A	91	GLU
1	A	97	GLU
1	A	103	SER
1	A	109	LEU
1	A	118	ASP
1	A	120	THR
1	A	122	LEU
1	A	127	GLN
1	A	136	LEU
1	A	146	LEU
1	A	152	ARG
1	A	159	ARG
1	A	185	MET
1	A	188	GLU
1	A	197	MET
1	A	206	LEU
1	A	208	LEU
1	A	217	THR
1	A	249	ASN
1	A	263	ARG
1	A	265	ILE
1	A	268	THR
1	A	286	SER
1	A	289	THR
1	A	290	LYS
1	A	296	VAL
1	A	306	LEU

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Mol	Chain	Res	Type
1	A	319	SER
1	A	330	GLU
1	A	332	ASP
1	A	339	LEU
1	A	343	LEU
1	A	352	LEU
1	A	361	LEU
1	A	370	LEU
1	A	376	ILE
1	A	395	GLU
1	A	400	LYS
1	A	417	LEU
1	A	421	MET
1	A	429	ASN
1	A	448	GLN
1	A	454	LYS
1	A	456	ASP
1	A	462	GLU
1	A	466	LEU
1	A	491	LEU
1	A	500	LYS
1	A	533	VAL
1	A	534	LEU
1	A	570	LYS
1	A	571	LEU
1	A	578	LEU
1	A	587	ARG
1	A	591	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	GLN
1	B	121	GLN
1	A	121	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	10/18 (55%)	6 (60%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	10/18 (55%)	7 (70%)	1 (10%)
All	All	20/36 (55%)	13 (65%)	1 (5%)

All (13) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	1141	G
2	C	1142	A
2	C	1144	U
2	C	1145	U
2	C	1146	G
2	C	1147	A
2	D	1141	G
2	D	1142	A
2	D	1143	A
2	D	1144	U
2	D	1145	U
2	D	1146	G
2	D	1150	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	1144	U

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	544/587 (92%)	-0.18	16 (2%)	55	47	15, 32, 60, 78	0
1	B	547/587 (93%)	-0.06	20 (3%)	45	37	16, 37, 69, 91	0
2	C	11/18 (61%)	1.12	2 (18%)	2	1	33, 44, 92, 103	0
2	D	11/18 (61%)	1.61	4 (36%)	0	0	44, 53, 114, 121	0
All	All	1113/1210 (91%)	-0.09	42 (3%)	44	36	15, 35, 67, 121	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1145	U	5.4
1	B	164	PRO	4.9
2	D	1144	U	4.9
2	C	1144	U	4.5
1	A	475	THR	4.5
1	B	249	ASN	4.1
1	B	75	ALA	3.8
1	A	316	ARG	3.6
1	A	164	PRO	3.6
1	B	477	ASP	3.5
2	D	1143	A	3.5
1	B	616	ARG	3.4
1	A	476	ARG	3.3
1	A	456	ASP	3.3
1	B	58	ARG	3.3
1	B	475	THR	3.2
1	B	282	ASP	3.2
1	B	476	ARG	3.2
1	A	454	LYS	3.0
1	B	478	ASP	3.0
1	A	477	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	58	ARG	2.8
1	A	249	ASN	2.8
1	B	176	VAL	2.8
1	A	220	ASN	2.8
2	C	1145	U	2.7
1	B	278	GLU	2.6
1	A	329	ASP	2.6
1	B	454	LYS	2.6
1	A	479	TRP	2.5
1	B	162	LEU	2.5
1	B	48	GLY	2.4
2	D	1140	G	2.4
1	A	278	GLU	2.4
1	A	77	GLU	2.3
1	B	316	ARG	2.2
1	B	74	ASP	2.1
1	B	453	GLU	2.1
1	B	59	GLU	2.0
1	A	59	GLU	2.0
1	A	455	SER	2.0
1	B	280	ARG	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.