Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:42 am BST

PDB ID	:	5N94
Title	:	Crystal Structure of Drosophila DHX36 helicase in complex with polyU
Authors	:	Chen, W.-F.; Rety, S.; Hai-Lei Guo, H.-L.; Wu, W.-Q.; Liu, N.-N.; Liu, Q.-W.; Dai, Y.-X.; Xi, X.-G.
Deposited on	:	2017-02-24
Resolution	:	2.43 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 following versions of software and data (see references ⓘ) were used in the production of this report:

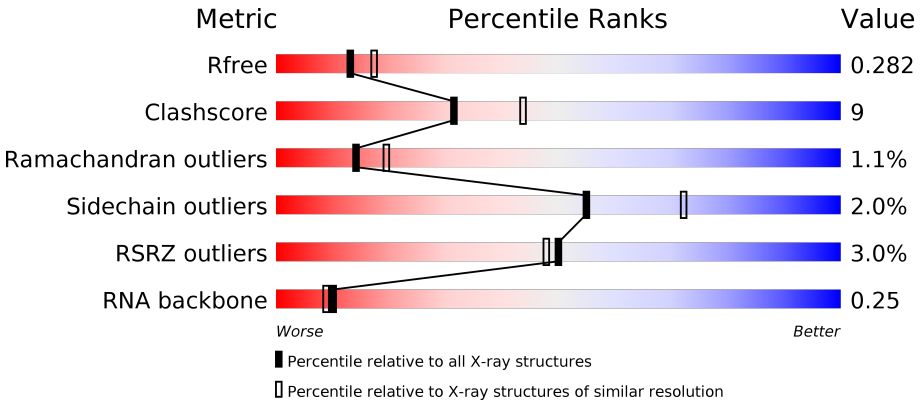
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.43 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)
RNA backbone	3102	1080 (2.80-2.04)

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 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 <=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	944	3% 72% 17% • 10%
1	B	944	3% 71% 17% • 10%
2	C	8	63% 25% 13%
2	D	8	38% 38% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14015 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 CG9323, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	849	Total	C	N	O	S	0	0	0
			6814	4304	1200	1265	45			
1	B	849	Total	C	N	O	S	0	0	0
			6814	4304	1200	1265	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	VAL	-	expression tag	UNP Q8SWT2
A	944	ASP	-	expression tag	UNP Q8SWT2
B	943	VAL	-	expression tag	UNP Q8SWT2
B	944	ASP	-	expression tag	UNP Q8SWT2

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			160	72	16	64	8			
2	D	8	Total	C	N	O	P	0	0	0
			160	72	16	64	8			

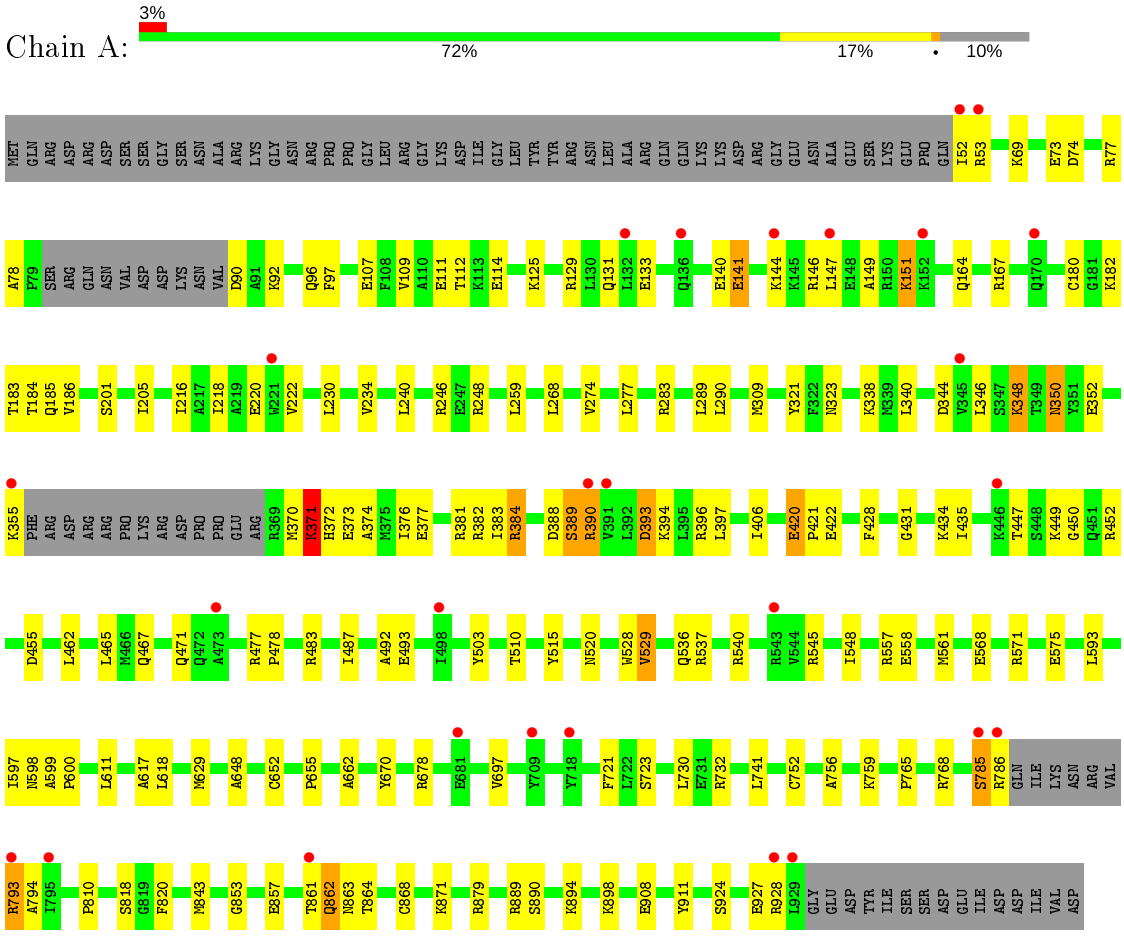
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	29	Total	O	0	0
			29	29		
3	C	4	Total	O	0	0
			4	4		
3	D	4	Total	O	0	0
			4	4		

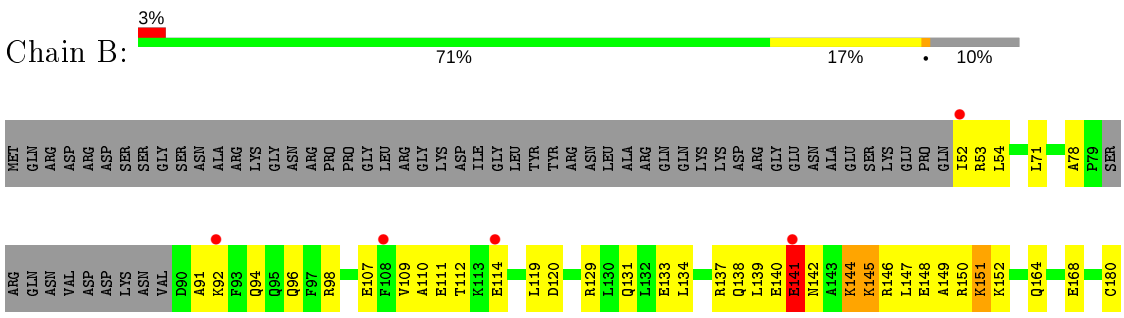
3 Residue-property plots (i)

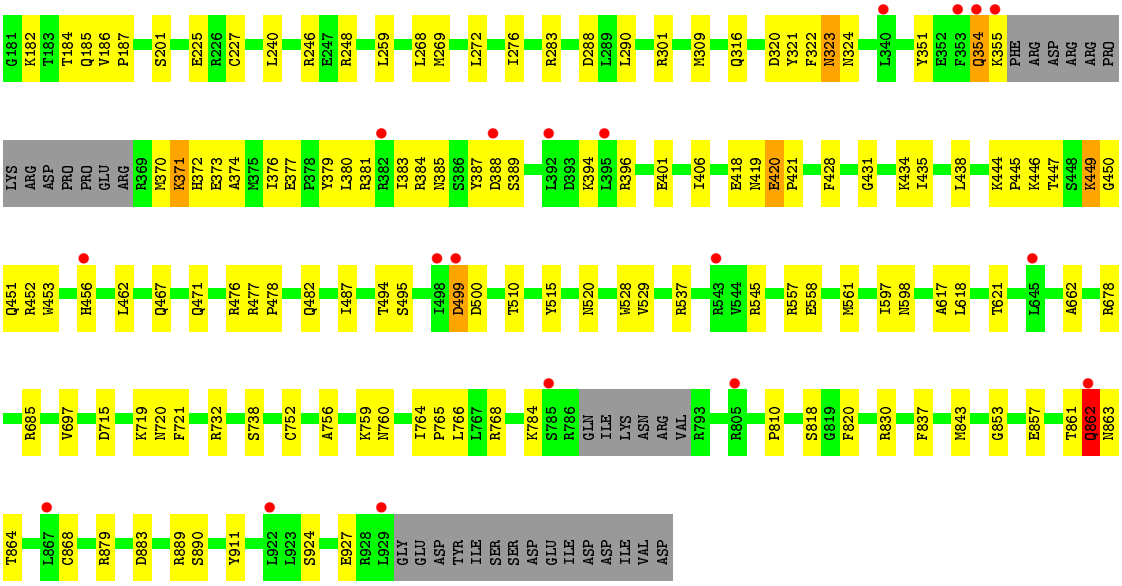
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: CG9323, isoform A



- Molecule 1: CG9323, isoform A



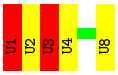


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain C:

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	338.33Å 51.53Å 159.90Å 90.00° 118.15° 90.00°	Depositor
Resolution (Å)	47.00 – 2.43 47.00 – 2.43	Depositor EDS
% Data completeness (in resolution range)	90.8 (47.00-2.43) 90.5 (47.00-2.43)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.212 , 0.278 0.219 , 0.282	Depositor DCC
R_{free} test set	4043 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.469 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14015	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.50	1/6933 (0.0%)	0.69	1/9353 (0.0%)
1	B	0.49	1/6933 (0.0%)	0.69	3/9353 (0.0%)
2	C	0.67	0/175	1.69	6/268 (2.2%)
2	D	0.71	0/175	1.60	7/268 (2.6%)
All	All	0.50	2/14216 (0.0%)	0.73	17/19242 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	752	CYS	CB-SG	-9.31	1.66	1.82
1	B	752	CYS	CB-SG	-5.31	1.73	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	U	C5-C6-N1	10.71	128.05	122.70
2	D	1	U	C5-C6-N1	8.22	126.81	122.70
2	D	1	U	C2-N1-C1'	7.08	126.20	117.70
2	C	1	U	C2-N1-C1'	6.98	126.08	117.70
2	D	3	U	C2-N1-C1'	6.82	125.89	117.70
2	C	3	U	C2-N1-C1'	6.35	125.32	117.70
1	B	862	GLN	CA-CB-CG	5.99	126.58	113.40
2	D	3	U	C6-N1-C1'	-5.46	113.56	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	355	LYS	CA-CB-CG	5.45	125.39	113.40
2	D	1	U	C6-N1-C1'	-5.43	113.59	121.20
2	C	1	U	N1-C2-N3	-5.42	111.64	114.90
1	A	371	LYS	N-CA-C	5.37	125.49	111.00
2	C	1	U	C2-N3-C4	5.36	130.22	127.00
1	B	141	GLU	N-CA-C	5.26	125.20	111.00
2	C	3	U	O4'-C1'-N1	5.24	112.39	108.20
2	D	1	U	N1-C2-N3	-5.18	111.79	114.90
2	D	3	U	N1-C2-O2	5.02	126.31	122.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	GLU	Peptide
1	A	390	ARG	Peptide
1	A	90	ASP	Peptide
1	B	141	GLU	Peptide
1	B	322	PHE	Peptide
1	B	354	GLN	Peptide
1	B	862	GLN	Peptide

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	6814	0	6913	126	0
1	B	6814	0	6913	123	0
2	C	160	0	81	6	0
2	D	160	0	81	4	0
3	A	30	0	0	3	0
3	B	29	0	0	1	0
3	C	4	0	0	0	0
3	D	4	0	0	1	0
All	All	14015	0	13988	250	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 9.

All (250) 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)
2:D:8:U:O3'	3:D:101:HOH:O	1.84	0.95
1:B:862:GLN:HB3	1:B:864:THR:H	1.33	0.91
1:B:283:ARG:NH2	1:B:598:ASN:OD1	2.02	0.91
1:A:373:GLU:HA	1:A:376:ILE:HG22	1.51	0.90
1:B:323:ASN:OD1	1:B:324:ASN:N	2.04	0.89
1:A:377:GLU:OE1	1:A:396:ARG:NH2	2.08	0.87
1:B:133:GLU:O	1:B:137:ARG:HG3	1.79	0.82
1:B:373:GLU:HA	1:B:376:ILE:HG22	1.59	0.82
1:A:390:ARG:CG	1:A:393:ASP:HB3	2.12	0.80
1:A:114:GLU:N	1:A:114:GLU:OE1	2.14	0.79
1:B:477:ARG:HG2	1:B:478:PRO:HD2	1.65	0.79
1:B:114:GLU:N	1:B:114:GLU:OE1	2.15	0.76
1:A:164:GLN:HE22	1:A:167:ARG:NH1	1.84	0.76
1:B:406:ILE:HD11	1:B:434:LYS:HD3	1.68	0.76
1:B:862:GLN:OE1	1:B:863:ASN:N	2.13	0.75
1:A:389:SER:OG	1:A:390:ARG:N	2.19	0.74
1:B:164:GLN:NE2	1:B:168:GLU:OE2	2.20	0.74
1:B:370:MET:HA	1:B:372:HIS:H	1.52	0.74
1:B:144:LYS:HA	1:B:147:LEU:HB3	1.70	0.73
1:A:393:ASP:OD1	1:A:394:LYS:N	2.22	0.72
1:A:390:ARG:HG3	1:A:393:ASP:HB3	1.69	0.72
1:A:393:ASP:CG	1:A:394:LYS:H	1.88	0.72
1:A:52:ILE:HD11	1:A:861:THR:HG21	1.71	0.71
1:B:765:PRO:HG2	1:B:927:GLU:HG2	1.73	0.71
1:B:418:GLU:HG2	1:B:453:TRP:HZ2	1.54	0.71
1:A:283:ARG:O	3:A:1001:HOH:O	2.08	0.70
1:A:449:LYS:HA	1:A:452:ARG:HD3	1.73	0.69
1:B:924:SER:O	1:B:927:GLU:HG3	1.92	0.69
1:A:810:PRO:HB2	2:C:1:U:C6	2.26	0.69
1:A:447:THR:HG22	1:A:450:GLY:H	1.58	0.69
1:B:853:GLY:O	1:B:889:ARG:NH2	2.26	0.68
1:B:379:TYR:O	1:B:383:ILE:HG22	1.94	0.68
1:B:381:ARG:O	1:B:384:ARG:HG3	1.94	0.68
1:A:393:ASP:CG	1:A:394:LYS:HG3	2.14	0.67
1:A:107:GLU:O	1:A:111:GLU:HG3	1.94	0.67
1:B:146:ARG:NH1	1:B:227:CYS:SG	2.68	0.67
1:B:351:TYR:O	1:B:394:LYS:NZ	2.24	0.67
1:A:131:GLN:OE1	3:A:1002:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:LYS:HB2	1:B:452:ARG:NH1	2.10	0.66
1:A:146:ARG:HA	1:A:149:ALA:HB3	1.78	0.66
1:A:862:GLN:OE1	1:A:863:ASN:N	2.28	0.66
1:B:370:MET:HA	1:B:372:HIS:N	2.09	0.66
1:B:146:ARG:HD3	1:B:225:GLU:HA	1.78	0.65
1:A:477:ARG:HH11	1:A:477:ARG:HG3	1.62	0.65
1:B:240:LEU:HD13	1:B:732:ARG:HB3	1.78	0.64
1:B:129:ARG:O	1:B:133:GLU:HG3	1.97	0.64
1:A:924:SER:O	1:A:927:GLU:HG3	1.98	0.63
1:B:449:LYS:HB2	1:B:452:ARG:HH12	1.61	0.63
1:B:857:GLU:HG2	1:B:868:CYS:SG	2.38	0.63
1:B:418:GLU:HG2	1:B:453:TRP:CZ2	2.34	0.63
1:A:259:LEU:HD23	1:A:290:LEU:HD21	1.82	0.62
1:B:447:THR:HG22	1:B:450:GLY:H	1.64	0.62
1:A:810:PRO:HB2	2:C:1:U:H6	1.63	0.62
1:A:129:ARG:O	1:A:133:GLU:HG3	2.00	0.61
1:B:377:GLU:OE1	1:B:396:ARG:NH1	2.30	0.61
1:B:467:GLN:OE1	1:B:471:GLN:NE2	2.27	0.61
1:A:515:TYR:OH	1:A:520:ASN:OD1	2.16	0.60
1:A:164:GLN:HE22	1:A:167:ARG:HH12	1.49	0.60
1:A:447:THR:HG22	1:A:450:GLY:N	2.15	0.60
1:B:499:ASP:N	1:B:499:ASP:OD1	2.32	0.60
1:A:406:ILE:HD11	1:A:434:LYS:HD3	1.83	0.60
1:B:112:THR:HG21	1:B:268:LEU:HD13	1.84	0.60
1:B:147:LEU:O	1:B:151:LYS:HG2	2.01	0.59
1:B:685:ARG:NH2	1:B:720:ASN:OD1	2.36	0.59
1:A:370:MET:HA	1:A:372:HIS:N	2.18	0.58
1:B:107:GLU:O	1:B:111:GLU:HG3	2.02	0.58
1:B:146:ARG:HA	1:B:149:ALA:HB3	1.85	0.58
1:B:145:LYS:HZ1	1:B:146:ARG:HG3	1.69	0.57
1:A:240:LEU:HD13	1:A:732:ARG:HB3	1.86	0.57
1:A:431:GLY:O	1:A:435:ILE:HG13	2.04	0.57
1:B:141:GLU:OE1	1:B:144:LYS:HG2	2.05	0.57
1:A:529:VAL:O	3:A:1003:HOH:O	2.17	0.56
1:A:756:ALA:O	1:A:759:LYS:HE3	2.06	0.56
1:A:467:GLN:OE1	1:A:471:GLN:NE2	2.35	0.56
1:A:283:ARG:NH2	1:A:598:ASN:OD1	2.33	0.56
1:B:148:GLU:O	1:B:152:LYS:HG3	2.05	0.56
1:B:91:ALA:HB1	1:B:94:GLN:H	1.71	0.56
1:A:449:LYS:HA	1:A:452:ARG:CD	2.36	0.55
1:A:759:LYS:NZ	1:A:908:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLY:O	1:B:435:ILE:HG13	2.07	0.55
1:B:383:ILE:HD11	1:B:387:TYR:CD2	2.41	0.55
1:A:69:LYS:O	1:A:73:GLU:HG3	2.07	0.55
1:A:381:ARG:O	1:A:383:ILE:N	2.40	0.54
1:A:370:MET:SD	1:A:373:GLU:HG2	2.48	0.54
1:B:756:ALA:O	1:B:759:LYS:NZ	2.31	0.54
1:B:142:ASN:HB2	1:B:145:LYS:HD3	1.90	0.54
1:B:377:GLU:O	1:B:381:ARG:HG3	2.08	0.54
1:B:445:PRO:HG2	1:B:451:GLN:HG2	1.89	0.54
1:B:447:THR:HG22	1:B:449:LYS:H	1.73	0.54
1:A:390:ARG:HG2	1:A:393:ASP:HB3	1.86	0.54
1:B:78:ALA:HB2	1:B:911:TYR:CG	2.44	0.54
1:A:109:VAL:HG22	1:A:268:LEU:HD21	1.90	0.53
1:A:390:ARG:HG3	1:A:393:ASP:CB	2.36	0.53
1:B:92:LYS:O	1:B:96:GLN:HG3	2.08	0.53
1:B:820:PHE:HB3	1:B:843:MET:SD	2.48	0.53
1:A:388:ASP:OD1	1:A:389:SER:N	2.42	0.53
1:A:492:ALA:O	1:A:540:ARG:NH1	2.42	0.53
1:B:477:ARG:CG	1:B:478:PRO:HD2	2.36	0.52
1:A:765:PRO:HG2	1:A:927:GLU:HG2	1.90	0.52
1:B:145:LYS:NZ	1:B:146:ARG:H	2.08	0.52
1:B:201:SER:O	1:B:248:ARG:NH1	2.41	0.52
1:A:340:LEU:HG	1:A:548:ILE:HD11	1.90	0.52
1:A:390:ARG:HE	1:A:393:ASP:HB3	1.73	0.52
1:A:393:ASP:OD2	1:A:394:LYS:HE3	2.09	0.52
1:A:112:THR:HG21	1:A:268:LEU:HD13	1.91	0.52
1:A:853:GLY:O	1:A:889:ARG:NH2	2.43	0.52
1:B:715:ASP:OD2	1:B:719:LYS:NZ	2.32	0.52
1:B:109:VAL:HG22	1:B:268:LEU:HD21	1.93	0.51
1:B:52:ILE:C	1:B:53:ARG:HD3	2.31	0.51
1:B:810:PRO:HG2	2:D:1:U:H1'	1.93	0.51
1:A:140:GLU:HG2	1:A:141:GLU:N	2.24	0.51
1:A:92:LYS:O	1:A:96:GLN:HG3	2.11	0.51
1:A:768:ARG:HD3	1:A:843:MET:O	2.11	0.50
1:B:134:LEU:O	1:B:138:GLN:HG3	2.11	0.50
1:A:820:PHE:HB3	1:A:843:MET:SD	2.52	0.49
1:A:467:GLN:HG3	1:A:670:TYR:CZ	2.48	0.49
1:B:371:LYS:O	1:B:374:ALA:N	2.45	0.49
1:B:131:GLN:OE1	3:B:1001:HOH:O	2.20	0.49
1:A:393:ASP:OD1	1:A:394:LYS:HG3	2.13	0.49
1:A:78:ALA:HB2	1:A:911:TYR:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASP:O	1:A:77:ARG:HG2	2.12	0.49
1:A:477:ARG:NH1	1:A:477:ARG:HG3	2.25	0.48
1:B:456:HIS:HA	1:B:482:GLN:HG2	1.95	0.48
1:B:617:ALA:O	1:B:618:LEU:HD23	2.14	0.48
1:B:810:PRO:HB2	2:D:1:U:C6	2.48	0.48
1:A:53:ARG:N	1:A:53:ARG:HD3	2.29	0.48
1:A:180:CYS:SG	1:A:182:LYS:HG2	2.53	0.48
1:A:371:LYS:O	1:A:374:ALA:N	2.46	0.48
1:A:421:PRO:HB2	1:A:545:ARG:HH22	1.78	0.47
1:A:186:VAL:HG21	1:A:309:MET:CE	2.44	0.47
2:D:3:U:H2'	2:D:4:U:O4'	2.15	0.47
1:B:186:VAL:HG21	1:B:309:MET:HE1	1.96	0.47
1:B:764:ILE:O	1:B:768:ARG:HG3	2.15	0.47
1:A:785:SER:OG	1:A:786:ARG:N	2.45	0.47
1:B:186:VAL:HG21	1:B:309:MET:CE	2.45	0.47
1:A:558:GLU:HA	1:A:561:MET:SD	2.55	0.47
1:B:184:THR:OG1	1:B:185:GLN:NE2	2.39	0.47
1:A:390:ARG:HE	1:A:393:ASP:CB	2.28	0.47
1:B:419:ASN:O	1:B:420:GLU:HB2	2.15	0.47
1:B:180:CYS:SG	1:B:182:LYS:HG2	2.54	0.46
1:B:428:PHE:CE2	1:B:537:ARG:HG2	2.50	0.46
1:B:447:THR:CG2	1:B:449:LYS:H	2.28	0.46
1:B:421:PRO:HB2	1:B:545:ARG:HH22	1.79	0.46
1:B:52:ILE:HD11	1:B:861:THR:HG21	1.96	0.46
1:B:381:ARG:O	1:B:383:ILE:N	2.49	0.46
1:B:528:TRP:CZ2	1:B:557:ARG:HD3	2.49	0.46
1:B:146:ARG:O	1:B:150:ARG:N	2.38	0.46
1:A:377:GLU:O	1:A:381:ARG:HG3	2.15	0.46
1:B:283:ARG:NH1	1:B:288:ASP:OD2	2.49	0.46
1:B:438:LEU:HD23	1:B:487:ILE:HG23	1.98	0.45
1:A:390:ARG:HG3	1:A:393:ASP:CA	2.46	0.45
1:B:371:LYS:NZ	1:B:557:ARG:HH22	2.14	0.45
1:A:394:LYS:HA	1:A:397:LEU:HG	1.98	0.45
1:A:617:ALA:O	1:A:618:LEU:HD23	2.17	0.45
1:A:125:LYS:NZ	1:B:120:ASP:OD1	2.39	0.45
1:B:376:ILE:O	1:B:380:LEU:HG	2.15	0.45
1:A:810:PRO:HB2	2:C:1:U:C5	2.51	0.45
1:B:383:ILE:HG12	1:B:383:ILE:O	2.16	0.45
1:B:494:THR:OG1	1:B:495:SER:N	2.50	0.45
1:A:205:ILE:HG12	1:A:274:VAL:HB	1.97	0.45
1:A:528:TRP:CE2	1:A:557:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASN:CB	1:B:145:LYS:HD3	2.46	0.45
1:B:447:THR:HG22	1:B:449:LYS:N	2.31	0.45
1:B:879:ARG:NH1	1:B:883:ASP:OD1	2.42	0.45
1:A:793:ARG:CG	1:A:794:ALA:N	2.80	0.45
1:A:857:GLU:HB2	1:A:871:LYS:HE2	1.99	0.45
1:A:201:SER:O	1:A:248:ARG:NH1	2.45	0.45
1:A:662:ALA:HB2	1:A:697:VAL:HG11	1.99	0.45
1:A:183:THR:HG21	1:A:218:ILE:HD13	1.99	0.44
1:A:477:ARG:HB3	1:A:478:PRO:HD2	1.99	0.44
1:A:52:ILE:C	1:A:53:ARG:HD3	2.37	0.44
1:A:670:TYR:CZ	1:A:723:SER:HB2	2.52	0.44
1:B:140:GLU:HG2	1:B:141:GLU:N	2.32	0.44
1:A:528:TRP:CZ2	1:A:557:ARG:HD3	2.53	0.44
1:B:71:LEU:HD23	1:B:71:LEU:HA	1.72	0.44
1:B:447:THR:HG22	1:B:450:GLY:N	2.29	0.44
1:B:138:GLN:O	1:B:139:LEU:HD23	2.17	0.44
1:B:388:ASP:OD1	1:B:389:SER:N	2.51	0.44
1:B:421:PRO:HB2	1:B:545:ARG:NH2	2.32	0.44
1:B:784:LYS:HD2	1:B:784:LYS:HA	1.81	0.44
1:B:515:TYR:OH	1:B:520:ASN:OD1	2.24	0.44
1:B:316:GLN:NE2	1:B:320:ASP:OD1	2.42	0.44
1:A:447:THR:CG2	1:A:449:LYS:H	2.30	0.43
1:B:144:LYS:HA	1:B:147:LEU:CB	2.45	0.43
1:B:558:GLU:HA	1:B:561:MET:SD	2.58	0.43
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.82	0.43
1:A:370:MET:HA	1:A:372:HIS:H	1.83	0.43
1:A:421:PRO:HB2	1:A:545:ARG:NH2	2.33	0.43
1:A:652:CYS:O	1:A:655:PRO:HD2	2.18	0.43
1:B:768:ARG:HD3	1:B:843:MET:O	2.17	0.43
1:A:810:PRO:CB	2:C:1:U:H6	2.30	0.43
1:A:147:LEU:O	1:A:151:LYS:HB2	2.18	0.43
1:A:428:PHE:CE2	1:A:537:ARG:HG2	2.53	0.43
1:B:269:MET:O	1:B:301:ARG:NH1	2.50	0.43
1:A:184:THR:OG1	1:A:185:GLN:NE2	2.46	0.43
1:A:420:GLU:HA	1:A:421:PRO:HD3	1.75	0.43
1:B:187:PRO:HG3	1:B:276:ILE:HD12	2.00	0.43
1:B:401:GLU:OE1	1:B:557:ARG:HD2	2.19	0.43
1:A:861:THR:HG23	1:A:862:GLN:N	2.34	0.43
1:B:52:ILE:HD11	1:B:861:THR:OG1	2.19	0.43
1:A:216:ILE:O	1:A:220:GLU:HG3	2.19	0.43
1:B:830:ARG:HA	1:B:837:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:ALA:HB2	1:B:697:VAL:HG11	2.01	0.43
1:B:678:ARG:HG2	1:B:721:PHE:HE2	1.83	0.43
1:A:862:GLN:OE1	1:A:864:THR:HG23	2.19	0.42
1:A:78:ALA:HB2	1:A:911:TYR:CG	2.54	0.42
1:B:760:ASN:HB3	1:B:766:LEU:HD23	2.02	0.42
1:B:145:LYS:HE2	1:B:146:ARG:HG3	2.02	0.42
1:A:493:GLU:HG2	1:A:536:GLN:HG2	2.01	0.42
1:B:107:GLU:O	1:B:110:ALA:HB3	2.20	0.42
1:B:377:GLU:O	1:B:377:GLU:HG3	2.19	0.42
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.92	0.42
1:A:421:PRO:HG2	1:A:545:ARG:HH22	1.84	0.42
1:A:277:LEU:HD21	1:A:290:LEU:HD23	2.02	0.42
1:A:503:TYR:HD1	1:A:548:ILE:HG22	1.84	0.42
1:B:246:ARG:HG3	1:B:248:ARG:O	2.20	0.42
1:A:422:GLU:HA	1:A:483:ARG:HH12	1.85	0.41
1:A:857:GLU:HB3	1:A:868:CYS:SG	2.60	0.41
1:A:97:PHE:HD1	1:A:629:MET:HE3	1.85	0.41
1:A:381:ARG:O	1:A:384:ARG:HG3	2.20	0.41
1:A:599:ALA:HA	1:A:600:PRO:HD3	1.91	0.41
1:B:500:ASP:OD1	1:B:500:ASP:N	2.54	0.41
1:A:246:ARG:HG3	1:A:248:ARG:O	2.20	0.41
1:A:862:GLN:O	1:A:863:ASN:ND2	2.54	0.41
1:B:110:ALA:O	1:B:114:GLU:OE1	2.39	0.41
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.88	0.41
1:A:730:LEU:HA	1:A:730:LEU:HD23	1.80	0.41
1:A:321:TYR:CD1	1:A:597:ILE:HG12	2.56	0.41
1:B:145:LYS:HZ1	1:B:146:ARG:H	1.68	0.41
1:B:321:TYR:CD1	1:B:597:ILE:HG12	2.55	0.41
1:B:421:PRO:HG2	1:B:545:ARG:HH22	1.84	0.41
1:A:394:LYS:H	1:A:394:LYS:HG3	1.71	0.41
1:A:503:TYR:CD1	1:A:548:ILE:HG22	2.56	0.41
1:A:678:ARG:HG2	1:A:721:PHE:HE2	1.85	0.41
1:A:648:ALA:HB2	1:A:741:LEU:HD23	2.03	0.41
1:A:344:ASP:O	1:A:348:LYS:HG3	2.21	0.41
1:A:810:PRO:HG2	2:C:1:U:H1'	2.03	0.41
1:B:462:LEU:HA	1:B:462:LEU:HD12	1.91	0.41
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.80	0.41
1:B:444:LYS:HG2	1:B:444:LYS:O	2.21	0.41
1:A:222:VAL:HG12	1:A:234:VAL:HG21	2.02	0.40
1:A:465:LEU:HD23	2:C:2:U:O2	2.20	0.40
1:B:145:LYS:NZ	1:B:146:ARG:HG3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:HD23	1:B:290:LEU:HD21	2.04	0.40
1:A:462:LEU:N	1:A:487:ILE:O	2.54	0.40
1:A:568:GLU:HA	1:A:571:ARG:HE	1.87	0.40
1:A:575:GLU:HG2	1:A:611:LEU:HD22	2.04	0.40
1:B:447:THR:O	1:B:451:GLN:HG3	2.21	0.40
1:A:593:LEU:HA	1:A:593:LEU:HD23	1.80	0.40
1:B:372:HIS:CG	1:B:372:HIS:O	2.74	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	841/944 (89%)	792 (94%)	38 (4%)	11 (1%)	12	16
1	B	841/944 (89%)	793 (94%)	41 (5%)	7 (1%)	19	27
All	All	1682/1888 (89%)	1585 (94%)	79 (5%)	18 (1%)	14	19

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ASN
1	A	371	LYS
1	A	389	SER
1	A	785	SER
1	B	323	ASN
1	B	371	LYS
1	B	862	GLN
1	A	144	LYS
1	A	323	ASN
1	A	393	ASP
1	A	382	ARG

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Mol	Chain	Res	Type
1	A	420	GLU
1	B	354	GLN
1	B	144	LYS
1	B	420	GLU
1	A	529	VAL
1	A	862	GLN
1	B	529	VAL

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	757/842 (90%)	741 (98%)	16 (2%)	53 71
1	B	757/842 (90%)	742 (98%)	15 (2%)	55 72
All	All	1514/1684 (90%)	1483 (98%)	31 (2%)	55 72

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	338	LYS
1	A	348	LYS
1	A	350	ASN
1	A	352	GLU
1	A	355	LYS
1	A	384	ARG
1	A	455	ASP
1	A	510	THR
1	A	793	ARG
1	A	818	SER
1	A	879	ARG
1	A	890	SER
1	A	894	LYS
1	A	898	LYS
1	A	928	ARG

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Mol	Chain	Res	Type
1	B	98	ARG
1	B	119	LEU
1	B	145	LYS
1	B	151	LYS
1	B	272	LEU
1	B	385	ASN
1	B	446	LYS
1	B	449	LYS
1	B	476	ARG
1	B	499	ASP
1	B	510	THR
1	B	621	THR
1	B	738	SER
1	B	818	SER
1	B	890	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	209	GLN
1	A	863	ASN
1	A	909	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	8/8 (100%)	2 (25%)	1 (12%)
2	D	8/8 (100%)	2 (25%)	1 (12%)
All	All	16/16 (100%)	4 (25%)	2 (12%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	U
2	C	3	U
2	D	2	U
2	D	3	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	1	U
2	D	1	U

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	849/944 (89%)	0.30	27 (3%) 47 45	37, 57, 90, 112	0
1	B	849/944 (89%)	0.25	24 (2%) 53 50	36, 57, 90, 108	0
2	C	8/8 (100%)	-0.07	0 100 100	43, 56, 71, 83	0
2	D	8/8 (100%)	-0.36	0 100 100	44, 58, 73, 83	0
All	All	1714/1904 (90%)	0.27	51 (2%) 50 48	36, 57, 90, 112	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	795	ILE	4.9
1	A	53	ARG	4.8
1	B	929	LEU	4.7
1	B	785	SER	4.3
1	A	543	ARG	3.8
1	B	355	LYS	3.8
1	A	785	SER	3.6
1	A	355	LYS	3.6
1	A	929	LEU	3.3
1	A	928	ARG	3.0
1	A	446	LYS	3.0
1	A	861	THR	3.0
1	B	108	PHE	3.0
1	B	805	ARG	3.0
1	B	456	HIS	3.0
1	A	793	ARG	2.9
1	A	681	GLU	2.7
1	A	709	TYR	2.7
1	A	52	ILE	2.7
1	B	354	GLN	2.7
1	B	392	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	395	LEU	2.7
1	A	718	TYR	2.6
1	B	340	LEU	2.6
1	B	114	GLU	2.6
1	B	52	ILE	2.5
1	A	144	LYS	2.5
1	A	498	ILE	2.4
1	A	390	ARG	2.4
1	B	382	ARG	2.4
1	B	645	LEU	2.4
1	A	391	VAL	2.3
1	A	147	LEU	2.3
1	B	353	PHE	2.3
1	A	345	VAL	2.2
1	A	221	TRP	2.2
1	A	152	LYS	2.2
1	A	786	ARG	2.2
1	A	136	GLN	2.2
1	B	92	LYS	2.2
1	B	388	ASP	2.2
1	B	498	ILE	2.2
1	B	499	ASP	2.1
1	A	132	LEU	2.1
1	B	867	LEU	2.1
1	B	922	LEU	2.1
1	B	141	GLU	2.1
1	A	170	GLN	2.0
1	B	862	GLN	2.0
1	B	543	ARG	2.0
1	A	473	ALA	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.