Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:58 pm BST

PDB ID	:	5N9D
Title	:	Crystal Structure of Drosophila DHX36 helicase in complex with GGGT-TAGGGT
Authors	:	Chen, W.-F.; Rety, S.; Guo, H.-L.; Wu, W.-Q.; Liu, N.-N.; Liu, Q.-W.; Dai, Y.-X.; Xi, X.-G.
Deposited on	:	2017-02-24
Resolution	:	2.71 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 ①) were used in the production of this report:

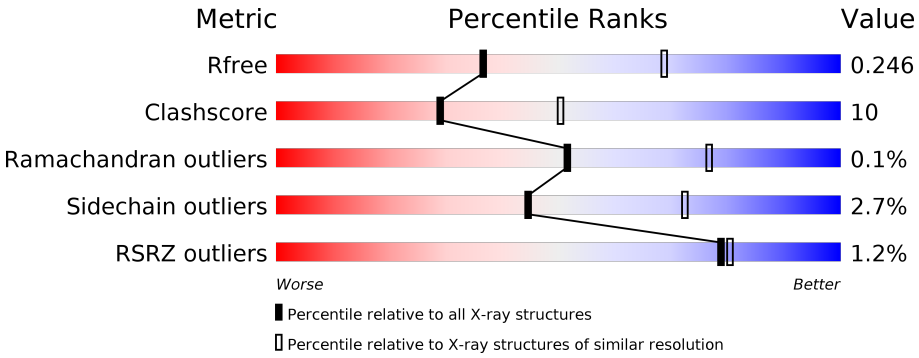
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	% 69% 20% • 9%
1	B	944	% 72% 19% • 8%
2	C	10	60% 40%
2	D	10	40% 50% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14301 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	855	Total	C	N	O	S	0	0	0
			6844	4322	1206	1271	45			
1	B	866	Total	C	N	O	S	0	0	0
			6904	4357	1217	1285	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 DNA chain called DNA (5'-D(P*GP*GP*GP*TP*TP*AP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	P	0	0	0
			213	100	41	62	10			
2	D	10	Total	C	N	O	P	0	0	0
			213	100	41	62	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	66	Total	O	0	0
			66	66		
3	C	5	Total	O	0	0
			5	5		

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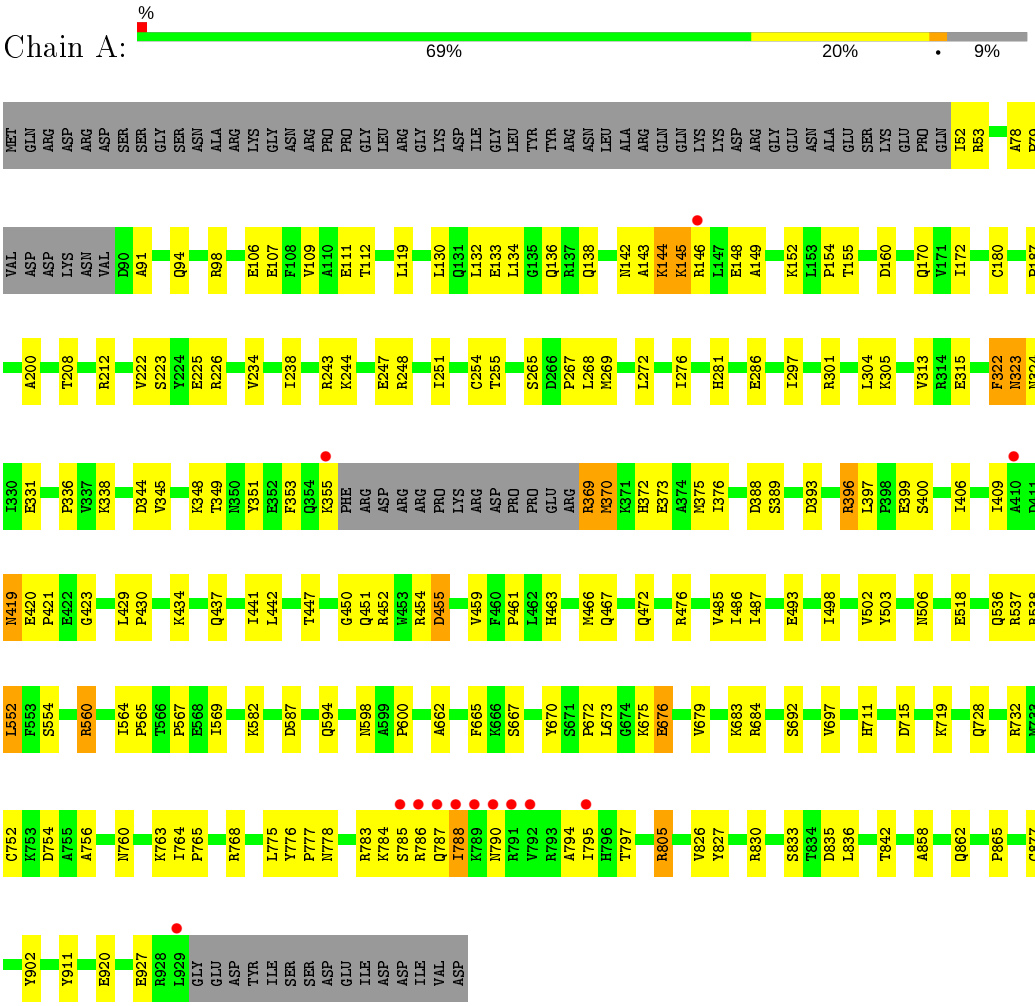
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total O 2 2	0	0

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 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.

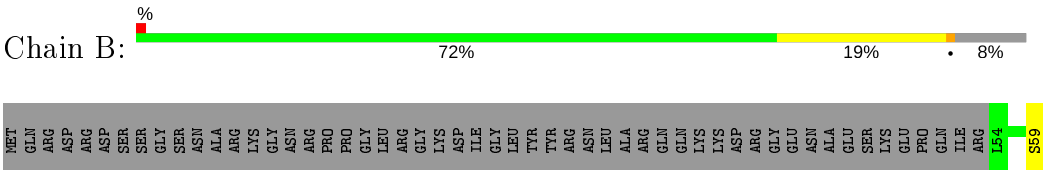
- Molecule 1: CG9323, isoform A

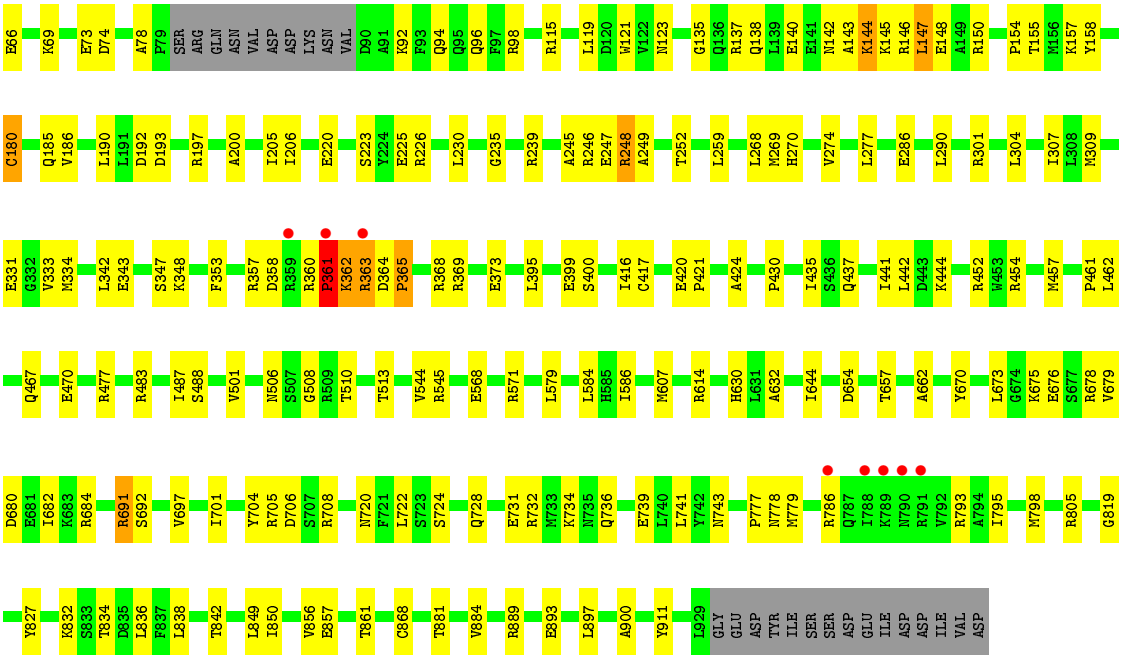
Chain A:



- Molecule 1: CG9323, isoform A

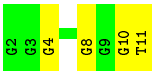
Chain B:





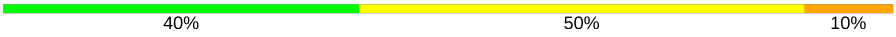
• Molecule 2: DNA (5'-D(P*GP*GP*GP*TP*TP*AP*GP*GP*GP*T)-3')

Chain C:



• Molecule 2: DNA (5'-D(P*GP*GP*GP*TP*TP*AP*GP*GP*GP*T)-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	305.44Å 51.34Å 164.95Å 90.00° 114.80° 90.00°	Depositor
Resolution (Å)	56.68 – 2.71 138.63 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.7 (56.68-2.71) 98.7 (138.63-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.69Å)	Xtriage
Refinement program	PHENIX (dev_2427: ???)	Depositor
R, R_{free}	0.185 , 0.247 0.185 , 0.246	Depositor DCC
R_{free} test set	3103 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14301	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 3.46% 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	0.46	0/6964	0.67	5/9398 (0.1%)
1	B	0.46	0/7027	0.68	4/9490 (0.0%)
2	C	0.97	0/239	1.02	0/369
2	D	1.19	0/239	1.08	1/369 (0.3%)
All	All	0.49	0/14469	0.69	10/19626 (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	10
1	B	0	6
All	All	0	16

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	361	PRO	N-CA-CB	8.24	113.19	103.30
1	A	455	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	322	PHE	C-N-CA	6.66	138.35	121.70
1	B	304	LEU	CB-CG-CD1	-6.23	100.40	111.00
1	A	552	LEU	CB-CG-CD2	-5.94	100.91	111.00
1	B	706	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	248	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	455	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	323	ASN	N-CA-C	5.27	125.22	111.00
2	D	5	DT	N3-C4-O4	5.13	122.98	119.90

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ASN	Peptide
1	A	144	LYS	Peptide
1	A	322	PHE	Peptide
1	A	323	ASN	Peptide
1	A	324	ASN	Peptide
1	A	370	MET	Peptide
1	A	421	PRO	Peptide
1	A	788	ILE	Peptide
1	A	790	ASN	Peptide
1	A	862	GLN	Peptide
1	B	144	LYS	Peptide
1	B	357	ARG	Peptide
1	B	363	ARG	Peptide
1	B	364	ASP	Peptide
1	B	365	PRO	Peptide
1	B	861	THR	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	6844	0	6926	144	0
1	B	6904	0	6948	120	0
2	C	213	0	114	4	0
2	D	213	0	114	8	0
3	A	54	0	0	8	0
3	B	66	0	0	7	0
3	C	5	0	0	0	0
3	D	2	0	0	4	0
All	All	14301	0	14102	270	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 10.

All (270) 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:760:ASN:OD1	1:A:763:LYS:NZ	1.85	1.10
1:A:461:PRO:HB2	1:A:466:MET:HE1	1.41	1.01
1:B:150:ARG:HE	1:B:185:GLN:HE22	1.09	0.95
1:B:358:ASP:O	1:B:361:PRO:N	2.03	0.92
1:B:786:ARG:HB2	1:B:795:ILE:HG12	1.53	0.90
1:B:343:GLU:HG3	1:B:395:LEU:HD21	1.54	0.90
1:A:52:ILE:N	3:A:1002:HOH:O	2.08	0.85
1:B:301:ARG:NH2	3:B:1001:HOH:O	1.99	0.85
1:A:786:ARG:HD2	1:A:788:ILE:H	1.39	0.84
1:A:146:ARG:HH12	1:A:149:ALA:HB3	1.44	0.81
1:A:437:GLN:O	3:A:1001:HOH:O	1.97	0.81
1:A:146:ARG:HH21	1:A:225:GLU:HG2	1.45	0.80
1:B:269:MET:O	1:B:301:ARG:NH1	2.15	0.79
1:A:463:HIS:HB3	1:A:466:MET:HG3	1.65	0.79
1:A:149:ALA:HA	1:A:152:LYS:HE3	1.66	0.78
1:B:157:LYS:O	3:B:1002:HOH:O	2.02	0.77
1:B:682:ILE:HD13	1:B:720:ASN:HA	1.68	0.76
1:A:373:GLU:HA	1:A:376:ILE:HG22	1.68	0.74
1:A:738:SER:OG	1:A:752:CYS:HB3	1.87	0.74
1:B:150:ARG:HE	1:B:185:GLN:NE2	1.86	0.73
1:A:370:MET:HA	1:A:372:HIS:H	1.53	0.73
1:B:150:ARG:NE	1:B:185:GLN:HE22	1.87	0.72
1:A:146:ARG:NH1	1:A:149:ALA:HB3	2.06	0.71
1:A:193:ASP:OD2	1:A:197:ARG:NH1	2.23	0.71
1:A:786:ARG:NH1	1:A:788:ILE:O	2.23	0.71
1:B:417:CYS:HA	1:B:483:ARG:HH11	1.55	0.70
1:A:375:MET:HG3	1:A:560:ARG:HD2	1.74	0.70
1:B:417:CYS:HA	1:B:483:ARG:NH1	2.07	0.69
1:B:239:ARG:HE	1:B:736:GLN:HE22	1.39	0.69
1:A:399:GLU:N	1:A:399:GLU:OE1	2.21	0.68
1:B:421:PRO:O	1:B:483:ARG:NH2	2.27	0.67
1:A:472:GLN:HG3	1:A:476:ARG:HD2	1.75	0.67
1:B:154:PRO:HG2	1:B:180:CYS:HA	1.77	0.67
1:A:370:MET:HA	1:A:372:HIS:N	2.10	0.66
1:A:784:LYS:HG2	1:A:797:THR:HB	1.79	0.65
1:A:388:ASP:OD2	1:A:389:SER:N	2.31	0.64
1:A:493:GLU:HG2	1:A:536:GLN:HG2	1.79	0.64
1:B:145:LYS:O	1:B:148:GLU:HB3	1.98	0.63
1:B:513:THR:HG23	3:B:1004:HOH:O	1.98	0.63
2:D:11:DT:C2	3:D:101:HOH:O	2.52	0.63
1:B:680:ASP:OD2	2:D:2:DG:N2	2.22	0.63
1:A:673:LEU:HD12	1:A:673:LEU:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ARG:CD	1:A:788:ILE:H	2.10	0.63
1:B:333:VAL:HG12	1:B:334:MET:O	1.99	0.62
1:A:134:LEU:O	1:A:138:GLN:HG3	1.99	0.62
2:D:11:DT:N3	3:D:101:HOH:O	2.28	0.62
1:A:281:HIS:HB2	1:A:313:VAL:HG22	1.81	0.62
1:B:644:ILE:HG22	1:B:741:LEU:HD11	1.81	0.62
1:B:193:ASP:OD2	1:B:197:ARG:NH1	2.33	0.62
1:B:399:GLU:N	1:B:399:GLU:OE1	2.21	0.61
1:B:121:TRP:O	1:B:248:ARG:NH2	2.34	0.61
1:B:65:LEU:HD22	1:B:884:VAL:HG11	1.83	0.60
1:A:268:LEU:HD23	1:A:297:ILE:HG12	1.82	0.60
2:D:11:DT:O2	3:D:101:HOH:O	2.16	0.60
1:B:705:ARG:HD3	1:B:731:GLU:OE2	2.02	0.59
1:B:143:ALA:HA	1:B:146:ARG:HB3	1.84	0.58
1:B:268:LEU:O	1:B:301:ARG:HD3	2.04	0.58
1:B:373:GLU:HG3	3:B:1039:HOH:O	2.04	0.58
1:A:423:GLY:HA3	1:A:502:VAL:CG2	2.33	0.58
2:D:6:DT:H2'	2:D:7:DA:H8	1.69	0.58
1:B:692:SER:HB2	1:B:842:THR:HG23	1.86	0.57
1:A:172:ILE:HG22	1:A:326:PRO:HG2	1.86	0.57
1:B:158:TYR:OH	1:B:331:GLU:OE2	2.20	0.57
1:A:286:GLU:N	1:A:286:GLU:OE1	2.35	0.56
1:A:132:LEU:O	1:A:136:GLN:HG3	2.05	0.56
1:A:786:ARG:HB3	1:A:794:ALA:HA	1.86	0.56
1:A:506:ASN:HB3	1:A:551:ASN:ND2	2.19	0.56
1:A:160:ASP:OD2	3:A:1003:HOH:O	2.16	0.56
1:A:351:TYR:HD2	1:A:353:PHE:CE2	2.23	0.56
1:A:419:ASN:HB2	1:A:420:GLU:HG2	1.88	0.56
1:B:675:LYS:NZ	1:B:678:ARG:HD3	2.20	0.56
1:B:691:ARG:NH1	1:B:819:GLY:O	2.38	0.56
1:A:397:LEU:HB3	1:A:399:GLU:OE1	2.05	0.56
1:B:724:SER:O	1:B:728:GLN:HG3	2.05	0.55
1:A:134:LEU:HG	1:A:138:GLN:NE2	2.21	0.55
1:A:442:LEU:HD12	1:A:487:ILE:HD11	1.87	0.55
1:B:205:ILE:HG12	1:B:274:VAL:CG1	2.36	0.55
1:B:657:THR:OG1	1:B:734:LYS:NZ	2.38	0.55
1:B:680:ASP:O	1:B:684:ARG:HG2	2.07	0.55
1:A:441:ILE:N	3:A:1001:HOH:O	2.40	0.55
1:A:805:ARG:NH1	1:A:835:ASP:OD2	2.40	0.55
1:A:715:ASP:OD1	1:A:719:LYS:NZ	2.28	0.54
1:B:92:LYS:O	1:B:96:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:OE2	3:A:1004:HOH:O	2.18	0.54
1:B:135:GLY:O	1:B:138:GLN:HG2	2.08	0.53
1:A:441:ILE:HG13	3:A:1001:HOH:O	2.08	0.53
1:A:783:ARG:O	1:A:784:LYS:HE2	2.08	0.53
1:B:190:LEU:HD11	1:B:307:ILE:HD11	1.91	0.53
1:B:220:GLU:HG3	1:B:230:LEU:HD22	1.91	0.53
2:D:5:DT:O2	3:D:102:HOH:O	2.17	0.52
1:A:234:VAL:HA	1:A:251:ILE:O	2.10	0.52
1:B:470:GLU:OE1	1:B:670:TYR:OH	2.18	0.52
1:B:654:ASP:OD2	1:B:705:ARG:NH2	2.43	0.52
1:A:784:LYS:HB2	1:A:797:THR:H	1.74	0.52
1:A:370:MET:CA	1:A:372:HIS:H	2.21	0.52
1:A:447:THR:HG23	1:A:450:GLY:H	1.75	0.52
1:B:146:ARG:HD3	3:B:1007:HOH:O	2.10	0.52
1:A:145:LYS:HG3	1:A:148:GLU:OE1	2.10	0.51
1:A:786:ARG:HD3	1:A:787:GLN:N	2.25	0.51
1:B:437:GLN:O	1:B:441:ILE:HD13	2.10	0.51
1:A:336:PRO:HD2	1:A:546:PRO:HG3	1.93	0.51
1:A:447:THR:O	1:A:451:GLN:HG3	2.11	0.51
1:A:304:LEU:HD12	1:A:305:LYS:H	1.76	0.51
1:A:393:ASP:O	1:A:396:ARG:HG3	2.10	0.51
1:A:567:PRO:CG	1:A:598:ASN:HD22	2.24	0.51
1:B:462:LEU:HB3	1:B:488:SER:HB2	1.92	0.51
1:A:281:HIS:HB2	1:A:313:VAL:CG2	2.41	0.51
1:A:486:ILE:HD13	1:A:498:ILE:HD13	1.92	0.50
1:A:506:ASN:HB3	1:A:551:ASN:HD22	1.76	0.50
1:B:78:ALA:HB2	1:B:911:TYR:CG	2.46	0.50
1:A:345:VAL:O	1:A:349:THR:HG22	2.12	0.50
1:A:582:LYS:NZ	1:A:587:ASP:O	2.44	0.50
1:B:94:GLN:HE21	1:B:98:ARG:HH21	1.57	0.50
1:B:365:PRO:HG2	1:B:368:ARG:HD3	1.93	0.50
1:A:134:LEU:C	1:A:138:GLN:HE21	2.15	0.50
1:A:212:ARG:HG3	2:C:8:DG:OP1	2.12	0.50
1:B:614:ARG:NH1	1:B:777:PRO:HG3	2.27	0.50
1:B:146:ARG:HD2	1:B:225:GLU:HA	1.93	0.49
1:B:342:LEU:HD21	1:B:400:SER:HB2	1.94	0.49
1:A:502:VAL:HG23	1:A:503:TYR:CD2	2.47	0.49
1:A:134:LEU:HG	1:A:138:GLN:HE21	1.77	0.49
1:B:424:ALA:HB3	1:B:501:VAL:HA	1.95	0.49
1:B:506:ASN:ND2	1:B:508:GLY:H	2.09	0.49
1:B:62:SER:O	1:B:66:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:MET:HE3	1:B:849:LEU:HD13	1.94	0.49
1:B:416:ILE:HG23	1:B:420:GLU:HG3	1.94	0.49
1:A:672:PRO:HG2	1:A:675:LYS:HB2	1.95	0.48
1:A:778:ASN:HB3	1:A:827:TYR:CZ	2.48	0.48
1:B:144:LYS:C	1:B:145:LYS:HD2	2.34	0.48
1:B:630:HIS:HE1	1:B:900:ALA:O	1.96	0.48
1:B:827:TYR:CG	1:B:838:LEU:HD22	2.48	0.48
1:A:567:PRO:HG3	1:A:598:ASN:ND2	2.28	0.48
1:A:765:PRO:HG2	1:A:927:GLU:HG2	1.95	0.48
1:B:277:LEU:HD21	1:B:290:LEU:HD13	1.94	0.48
1:B:348:LYS:NZ	3:B:1012:HOH:O	2.46	0.48
1:A:369:ARG:HA	1:A:369:ARG:NE	2.29	0.48
1:A:79:PRO:O	3:A:1005:HOH:O	2.20	0.48
1:A:594:GLN:NE2	3:A:1008:HOH:O	2.45	0.48
1:B:893:GLU:O	1:B:897:LEU:HD22	2.13	0.47
1:B:142:ASN:O	1:B:146:ARG:HB2	2.13	0.47
1:B:739:GLU:O	1:B:743:ASN:ND2	2.46	0.47
1:B:461:PRO:HG3	1:B:673:LEU:HD12	1.96	0.47
1:B:200:ALA:HB1	1:B:249:ALA:HB2	1.96	0.47
1:B:259:LEU:HD23	1:B:290:LEU:HD11	1.97	0.47
1:A:107:GLU:O	1:A:111:GLU:HG3	2.14	0.47
1:A:146:ARG:HH11	1:A:146:ARG:HA	1.80	0.47
1:B:145:LYS:N	1:B:145:LYS:HD2	2.29	0.47
1:B:676:GLU:O	1:B:679:VAL:HG12	2.14	0.47
1:A:338:LYS:HB3	1:A:338:LYS:HE2	1.54	0.47
1:A:455:ASP:OD1	1:A:455:ASP:O	2.32	0.47
1:B:286:GLU:OE2	1:B:286:GLU:N	2.45	0.47
1:B:467:GLN:HG3	1:B:670:TYR:CZ	2.49	0.47
1:B:544:VAL:HG23	1:B:545:ARG:HG2	1.97	0.46
1:B:793:ARG:NH1	3:B:1014:HOH:O	2.47	0.46
1:A:778:ASN:HB3	1:A:827:TYR:CE2	2.49	0.46
1:B:235:GLY:N	1:B:245:ALA:HB2	2.30	0.46
1:B:857:GLU:HG2	1:B:868:CYS:SG	2.55	0.46
2:D:6:DT:H2'	2:D:7:DA:C8	2.49	0.46
1:A:467:GLN:HG3	1:A:670:TYR:CZ	2.50	0.46
1:B:701:ILE:O	1:B:705:ARG:HG3	2.16	0.46
1:B:779:MET:CE	1:B:849:LEU:HD13	2.46	0.46
1:B:728:GLN:O	1:B:732:ARG:HG3	2.16	0.46
1:B:778:ASN:HB3	1:B:827:TYR:CZ	2.51	0.46
1:B:92:LYS:HD3	1:B:92:LYS:HA	1.66	0.46
1:A:130:LEU:HD12	1:A:200:ALA:HB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLY:HA3	1:A:502:VAL:HG22	1.97	0.45
1:B:893:GLU:O	1:B:897:LEU:CD2	2.64	0.45
1:A:692:SER:HB2	1:A:842:THR:HG23	1.98	0.45
1:B:144:LYS:HA	1:B:147:LEU:HB3	1.99	0.45
1:B:360:ARG:C	1:B:362:LYS:H	2.20	0.45
1:A:764:ILE:O	1:A:768:ARG:HG3	2.16	0.45
1:B:145:LYS:HA	1:B:148:GLU:HB2	1.99	0.45
1:A:676:GLU:O	1:A:679:VAL:HG12	2.16	0.45
1:A:786:ARG:HB3	1:A:795:ILE:H	1.81	0.45
1:A:146:ARG:NH1	1:A:146:ARG:HA	2.32	0.45
1:A:412:LEU:O	1:A:416:ILE:HG13	2.17	0.45
1:B:186:VAL:HG21	1:B:309:MET:HE2	1.97	0.45
1:A:98:ARG:HG3	1:A:98:ARG:HH11	1.81	0.45
1:B:192:ASP:OD1	1:B:226:ARG:NH2	2.50	0.45
1:A:344:ASP:O	1:A:348:LYS:HG2	2.15	0.45
1:A:78:ALA:HB2	1:A:911:TYR:CG	2.52	0.45
1:B:832:LYS:HB2	1:B:836:LEU:HD13	1.99	0.45
1:B:675:LYS:HZ3	1:B:678:ARG:HD3	1.80	0.44
1:B:798:MET:O	1:B:805:ARG:HG2	2.17	0.44
1:A:502:VAL:HG23	1:A:503:TYR:CE2	2.52	0.44
1:A:673:LEU:HD12	1:A:673:LEU:N	2.32	0.44
1:A:776:TYR:CG	1:A:777:PRO:HA	2.52	0.44
1:B:137:ARG:NH1	1:B:226:ARG:O	2.51	0.44
1:A:91:ALA:HB2	1:A:902:TYR:HD1	1.83	0.44
1:A:679:VAL:HG22	1:A:683:LYS:HD2	1.99	0.44
1:B:442:LEU:HB3	1:B:457:MET:HE1	1.98	0.44
1:B:430:PRO:HA	1:B:510:THR:HA	1.99	0.44
1:B:270:HIS:HA	1:B:301:ARG:NH1	2.33	0.44
1:B:137:ARG:HG3	1:B:140:GLU:OE2	2.17	0.44
1:A:145:LYS:HE2	1:A:148:GLU:CD	2.38	0.44
1:A:353:PHE:HE1	1:A:400:SER:HB3	1.82	0.44
1:A:459:VAL:HG22	1:A:485:VAL:HB	2.00	0.44
1:A:208:THR:HA	1:A:254:CYS:O	2.18	0.43
1:B:579:LEU:HG	1:B:632:ALA:HB2	2.00	0.43
1:A:409:ILE:HG22	1:A:552:LEU:HD21	1.99	0.43
1:B:363:ARG:O	1:B:365:PRO:HD3	2.19	0.43
1:A:265:SER:OG	2:C:10:DG:O6	2.27	0.43
1:A:406:ILE:O	1:A:409:ILE:HG13	2.18	0.43
1:B:584:LEU:O	1:B:586:ILE:HD12	2.19	0.43
1:B:850:ILE:O	1:B:889:ARG:HD2	2.18	0.43
1:A:143:ALA:C	1:A:145:LYS:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:OG1	1:A:180:CYS:O	2.26	0.43
1:B:144:LYS:O	1:B:145:LYS:HD2	2.18	0.43
1:A:662:ALA:HB2	1:A:697:VAL:HG11	2.02	0.42
1:A:351:TYR:HD2	1:A:353:PHE:CD2	2.36	0.42
1:A:830:ARG:HD2	1:A:836:LEU:HD21	2.02	0.42
1:A:315:GLU:OE2	1:A:329:ARG:NH2	2.52	0.42
1:A:728:GLN:O	1:A:732:ARG:HG3	2.20	0.42
1:A:784:LYS:HG2	1:A:797:THR:CB	2.47	0.42
1:A:786:ARG:HD2	1:A:788:ILE:N	2.20	0.42
1:A:784:LYS:HB2	1:A:797:THR:N	2.34	0.42
1:B:230:LEU:HA	1:B:230:LEU:HD12	1.83	0.42
1:B:206:ILE:HD13	1:B:252:THR:HB	2.01	0.42
1:B:722:LEU:HD23	1:B:722:LEU:HA	1.81	0.42
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.85	0.42
1:A:238:ILE:HG22	1:A:255:THR:HG23	2.02	0.42
1:A:154:PRO:HB3	1:A:331:GLU:HG2	2.01	0.42
1:B:704:TYR:CZ	1:B:708:ARG:HD2	2.54	0.42
1:A:119:LEU:HD23	1:A:248:ARG:CZ	2.50	0.42
1:A:269:MET:HB3	1:A:272:LEU:HD21	2.01	0.42
1:A:244:LYS:NZ	2:C:11:DT:H5"	2.35	0.42
1:B:778:ASN:HB3	1:B:827:TYR:CE2	2.55	0.42
1:A:187:PRO:HG3	1:A:276:ILE:HD13	2.02	0.42
1:A:143:ALA:O	1:A:144:LYS:HB3	2.19	0.42
1:A:775:LEU:HD12	1:A:826:VAL:HG23	2.02	0.42
1:A:112:THR:OG1	1:A:267:PRO:HD2	2.20	0.42
1:A:406:ILE:HD11	1:A:434:LYS:NZ	2.35	0.42
1:B:834:THR:HG21	2:D:3:DG:OP1	2.20	0.42
1:A:833:SER:OG	2:C:4:DG:OP1	2.34	0.41
1:A:858:ALA:HB1	1:A:879:ARG:HH12	1.86	0.41
1:A:243:ARG:N	1:A:243:ARG:HD3	2.35	0.41
1:B:69:LYS:O	1:B:73:GLU:HG3	2.20	0.41
1:A:734:LYS:HG2	1:A:734:LYS:HZ2	1.70	0.41
1:B:119:LEU:HA	1:B:119:LEU:HD23	1.86	0.41
1:B:155:THR:OG1	1:B:180:CYS:O	2.18	0.41
1:A:567:PRO:CG	1:A:598:ASN:ND2	2.83	0.41
1:B:856:VAL:HA	1:B:868:CYS:O	2.19	0.41
1:A:146:ARG:HH21	1:A:225:GLU:CG	2.23	0.41
1:A:170:GLN:NE2	1:A:301:ARG:O	2.53	0.41
1:A:569:ILE:HG13	1:A:600:PRO:HG3	2.02	0.41
1:A:711:HIS:N	1:A:711:HIS:CD2	2.88	0.41
1:B:247:GLU:HG3	1:B:248:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:ALA:HB2	1:B:697:VAL:HG11	2.02	0.41
1:A:212:ARG:HB3	1:A:238:ILE:HD12	2.02	0.41
1:A:109:VAL:HA	1:A:112:THR:HG22	2.01	0.41
1:A:351:TYR:HD2	1:A:353:PHE:HE2	1.69	0.41
1:B:353:PHE:CZ	1:B:400:SER:HA	2.56	0.41
1:A:145:LYS:HE2	1:A:148:GLU:HG2	2.02	0.41
1:B:246:ARG:HH21	1:B:249:ALA:CB	2.33	0.41
1:B:568:GLU:HG3	1:B:571:ARG:NH2	2.36	0.41
1:A:145:LYS:HA	1:A:148:GLU:HG3	2.01	0.41
1:A:429:LEU:HB3	1:A:430:PRO:HD2	2.02	0.41
1:B:137:ARG:O	1:B:137:ARG:HG2	2.21	0.41
1:B:442:LEU:HD22	1:B:457:MET:HE1	2.03	0.41
1:A:345:VAL:HG21	1:A:412:LEU:HD22	2.03	0.40
1:A:409:ILE:HD13	1:A:409:ILE:HG21	1.93	0.40
1:A:564:ILE:HG13	1:A:565:PRO:O	2.22	0.40
1:A:754:ASP:OD2	1:A:756:ALA:HB3	2.21	0.40
1:A:145:LYS:O	1:A:148:GLU:HG3	2.21	0.40
1:B:65:LEU:CD2	1:B:884:VAL:HG11	2.51	0.40
1:A:865:PRO:HB2	1:A:877:CYS:O	2.21	0.40
1:B:435:ILE:HG12	1:B:487:ILE:HG22	2.02	0.40
1:A:222:VAL:O	1:A:226:ARG:HG3	2.22	0.40
1:B:881:THR:O	1:B:884:VAL:HG12	2.21	0.40
1:B:119:LEU:HD23	1:B:248:ARG:CZ	2.52	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	849/944 (90%)	832 (98%)	17 (2%)	0	100 100
1	B	862/944 (91%)	845 (98%)	15 (2%)	2 (0%)	47 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1711/1888 (91%)	1677 (98%)	32 (2%)	2 (0%)	51 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	PRO
1	B	362	LYS

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	757/842 (90%)	731 (97%)	26 (3%)	37 65
1	B	759/842 (90%)	744 (98%)	15 (2%)	55 80
All	All	1516/1684 (90%)	1475 (97%)	41 (3%)	44 72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	94	GLN
1	A	106	GLU
1	A	133	GLU
1	A	145	LYS
1	A	223	SER
1	A	355	LYS
1	A	369	ARG
1	A	396	ARG
1	A	419	ASN
1	A	452	ARG
1	A	454	ARG
1	A	518	GLU
1	A	537	ARG
1	A	538	ARG
1	A	554	SER

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Mol	Chain	Res	Type
1	A	560	ARG
1	A	665	PHE
1	A	667	SER
1	A	676	GLU
1	A	684	ARG
1	A	785	SER
1	A	805	ARG
1	A	879	ARG
1	A	890	SER
1	A	920	GLU
1	B	59	SER
1	B	74	ASP
1	B	115	ARG
1	B	123	ASN
1	B	147	LEU
1	B	180	CYS
1	B	223	SER
1	B	347	SER
1	B	369	ARG
1	B	444	LYS
1	B	452	ARG
1	B	454	ARG
1	B	477	ARG
1	B	607	MET
1	B	691	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	131	GLN
1	A	138	GLN
1	A	164	GLN
1	A	170	GLN
1	A	551	ASN
1	A	598	ASN
1	A	711	HIS
1	B	123	ASN
1	B	138	GLN
1	B	185	GLN
1	B	467	GLN
1	B	506	ASN

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Mol	Chain	Res	Type
1	B	630	HIS
1	B	736	GLN
1	B	743	ASN
1	B	781	HIS

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

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	855/944 (90%)	0.02	13 (1%) 73 76	28, 57, 106, 133	0
1	B	866/944 (91%)	-0.06	8 (0%) 84 85	29, 54, 95, 136	0
2	C	10/10 (100%)	0.21	0 100 100	52, 76, 94, 100	0
2	D	10/10 (100%)	-0.00	0 100 100	45, 65, 79, 90	0
All	All	1741/1908 (91%)	-0.02	21 (1%) 79 80	28, 55, 101, 136	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	790	ASN	8.1
1	A	791	ARG	6.8
1	A	792	VAL	6.7
1	A	788	ILE	6.0
1	A	786	ARG	4.5
1	A	785	SER	3.7
1	B	786	ARG	3.6
1	A	355	LYS	3.3
1	B	359	ARG	3.1
1	A	929	LEU	3.1
1	B	791	ARG	3.0
1	A	789	LYS	2.8
1	A	787	GLN	2.7
1	B	790	ASN	2.7
1	A	795	ILE	2.6
1	B	361	PRO	2.6
1	B	789	LYS	2.2
1	A	410	ALA	2.2
1	A	146	ARG	2.2
1	B	363	ARG	2.1
1	B	788	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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.