Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 03:51 AM EDT

PDB ID	:	5N8R
Title	:	Crystal Structure of Drosophilia DHX36 helicase in complex with GAG-CACTGC
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	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

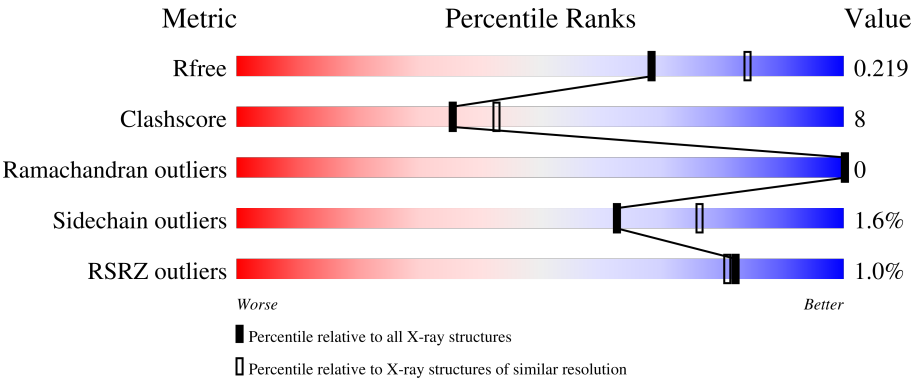
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 74% 15% • 10%
1	B	944	% 76% 13% • 10%
2	C	9	33% 56% 11%
2	D	9	33% 67%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14846 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	851	Total	C	N	O	S	0	0	0
			6829	4312	1202	1270	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*AP*GP*CP*AP*CP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			185	87	36	53	9			
2	D	9	Total	C	N	O	P	0	0	0
			185	87	36	53	9			

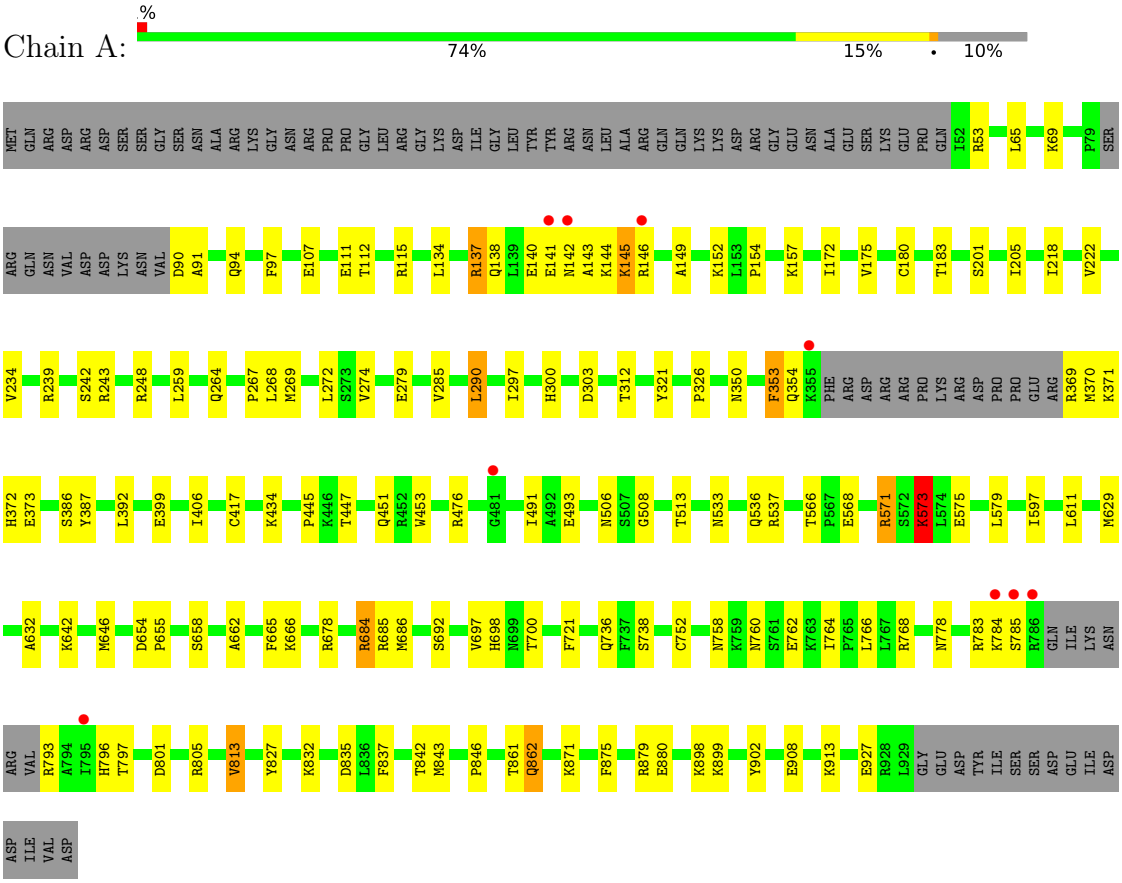
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	377	Total	O	0	0
			377	377		
3	B	424	Total	O	0	0
			424	424		
3	C	14	Total	O	0	0
			14	14		
3	D	18	Total	O	0	0
			18	18		

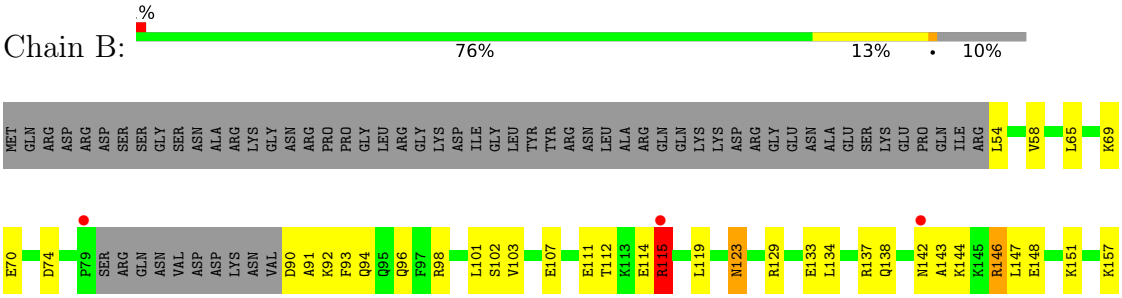
3 Residue-property plots (i)

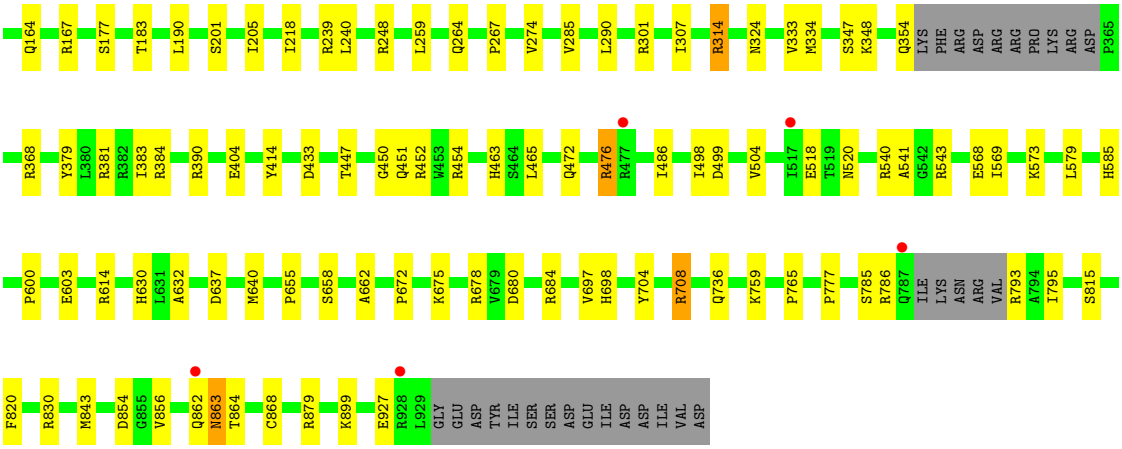
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CG9323, isoform A



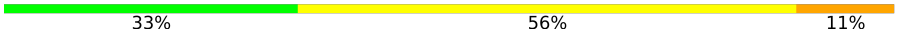
• Molecule 1: CG9323, isoform A

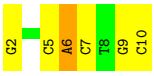




• Molecule 2: DNA (5'-D(P*GP*AP*GP*CP*AP*CP*TP*GP*C)-3')

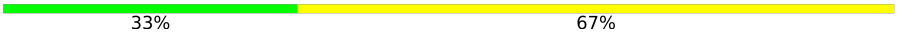
Chain C:





• Molecule 2: DNA (5'-D(P*GP*AP*GP*CP*AP*CP*TP*GP*C)-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	300.87Å 51.48Å 164.39Å 90.00° 114.22° 90.00°	Depositor
Resolution (Å)	149.90 – 2.20 149.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (149.90-2.20) 99.3 (149.92-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.176 , 0.219 0.176 , 0.219	Depositor DCC
R_{free} test set	5865 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14846	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.49	5/6933 (0.1%)	0.69	7/9353 (0.1%)
1	B	0.45	0/6950	0.66	1/9378 (0.0%)
2	C	1.00	0/207	0.97	1/317 (0.3%)
2	D	1.12	0/207	1.06	1/317 (0.3%)
All	All	0.50	5/14297 (0.0%)	0.69	10/19365 (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	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	880	GLU	CD-OE1	-7.47	1.17	1.25
1	A	145	LYS	CD-CE	-7.29	1.33	1.51
1	A	684	ARG	CD-NE	-6.18	1.35	1.46
1	A	573	LYS	CD-CE	5.63	1.65	1.51
1	A	684	ARG	CZ-NH2	5.43	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	684	ARG	NE-CZ-NH1	-10.40	115.10	120.30
1	A	145	LYS	CD-CE-NZ	-10.01	88.69	111.70
1	A	571	ARG	CG-CD-NE	6.61	125.67	111.80
2	D	6	DA	O4'-C4'-C3'	-6.34	101.97	104.50
1	B	115	ARG	CD-NE-CZ	5.91	131.87	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	880	GLU	N-CA-CB	-5.86	100.06	110.60
2	C	6	DA	O4'-C4'-C3'	-5.39	102.34	104.50
1	A	880	GLU	CA-CB-CG	5.23	124.91	113.40
1	A	813	VAL	CG1-CB-CG2	5.12	119.09	110.90
1	A	145	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	PHE	Peptide
1	A	783	ARG	Peptide
1	B	115	ARG	Sidechain

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	127	0
1	B	6829	0	6918	96	2
2	C	185	0	101	8	0
2	D	185	0	101	7	0
3	A	377	0	0	20	0
3	B	424	0	0	21	0
3	C	14	0	0	0	0
3	D	18	0	0	2	0
All	All	14846	0	14033	228	2

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 8.

All (228) 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:142:ASN:N	1:A:145:LYS:HZ3	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LYS:HG2	1:A:796:HIS:HA	1.38	1.05
1:A:476:ARG:NH1	3:A:1004:HOH:O	1.95	0.98
1:A:566:THR:O	1:A:571:ARG:NH1	1.97	0.96
1:A:927:GLU:O	3:A:1001:HOH:O	1.82	0.96
1:B:637:ASP:OD1	3:B:1001:HOH:O	1.88	0.92
1:A:279:GLU:OE2	3:A:1002:HOH:O	1.90	0.90
1:A:685:ARG:NH1	3:A:1005:HOH:O	2.05	0.89
1:B:678:ARG:HG2	3:B:1392:HOH:O	1.72	0.89
1:A:142:ASN:CA	1:A:145:LYS:HZ3	1.88	0.87
1:B:463:HIS:HD2	1:B:465:LEU:H	1.21	0.86
1:B:499:ASP:OD2	1:B:543:ARG:NH1	2.09	0.85
1:B:573:LYS:NZ	3:B:1005:HOH:O	2.11	0.83
1:B:786:ARG:HB2	1:B:795:ILE:HG22	1.61	0.82
1:B:354:GLN:O	3:B:1002:HOH:O	1.99	0.81
1:A:142:ASN:N	1:A:145:LYS:NZ	2.28	0.81
1:A:654:ASP:H	1:A:758:ASN:HD21	1.28	0.80
1:A:666:LYS:NZ	3:A:1003:HOH:O	1.92	0.79
1:A:832:LYS:NZ	3:A:1011:HOH:O	2.16	0.78
2:D:3:DA:OP2	3:D:101:HOH:O	2.00	0.78
1:B:433:ASP:OD1	3:B:1003:HOH:O	2.03	0.77
1:B:759:LYS:NZ	3:B:1010:HOH:O	2.17	0.77
1:B:447:THR:HG23	1:B:450:GLY:H	1.51	0.74
1:A:145:LYS:H	1:A:145:LYS:HD2	1.51	0.74
1:B:447:THR:HG22	3:B:1196:HOH:O	1.86	0.74
1:B:862:GLN:CD	1:B:863:ASN:H	1.90	0.74
1:A:573:LYS:HG3	1:A:575:GLU:OE1	1.87	0.73
1:A:386:SER:OG	3:A:1006:HOH:O	2.06	0.73
1:A:303:ASP:O	3:A:1007:HOH:O	2.08	0.71
1:B:239:ARG:HE	1:B:736:GLN:HE22	1.39	0.71
1:A:370:MET:SD	1:A:370:MET:N	2.64	0.71
1:A:285:VAL:HG23	1:A:568:GLU:HG3	1.74	0.69
1:B:368:ARG:NH2	1:B:404:GLU:OE2	2.24	0.69
1:A:137:ARG:HA	1:A:140:GLU:HG3	1.75	0.69
1:B:264:GLN:HB2	2:D:10:DC:N4	2.08	0.69
1:B:144:LYS:O	1:B:147:LEU:N	2.17	0.68
1:B:107:GLU:O	1:B:111:GLU:HG3	1.94	0.67
1:A:259:LEU:HD23	1:A:290:LEU:HD11	1.76	0.67
1:B:133:GLU:OE1	3:B:1007:HOH:O	2.12	0.67
1:B:285:VAL:HG23	1:B:568:GLU:HG2	1.75	0.67
2:D:9:DG:N7	3:D:102:HOH:O	2.28	0.67
1:A:141:GLU:HA	1:A:145:LYS:HZ1	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:ASN:HB3	1:A:766:LEU:HD23	1.78	0.66
1:A:784:LYS:CB	1:A:797:THR:H	2.09	0.65
1:A:533:ASN:OD1	3:A:1008:HOH:O	2.13	0.65
1:B:862:GLN:OE1	1:B:864:THR:N	2.30	0.65
1:A:784:LYS:HD3	1:A:785:SER:H	1.62	0.64
1:B:862:GLN:OE1	1:B:864:THR:OG1	2.05	0.64
1:B:91:ALA:HB1	3:B:1071:HOH:O	1.98	0.64
1:B:463:HIS:HE1	2:D:5:DC:OP2	1.78	0.64
1:B:348:LYS:NZ	3:B:1004:HOH:O	2.09	0.64
1:A:145:LYS:HD2	1:A:145:LYS:N	2.12	0.63
1:A:172:ILE:HG22	1:A:326:PRO:HG2	1.79	0.63
1:A:350:ASN:OD1	3:A:1009:HOH:O	2.16	0.63
1:A:762:GLU:OE1	3:A:1010:HOH:O	2.16	0.63
1:A:141:GLU:C	1:A:145:LYS:HZ3	2.02	0.62
1:B:486:ILE:HD13	1:B:498:ILE:HD13	1.81	0.62
1:A:146:ARG:NH1	1:A:149:ALA:HB3	2.14	0.62
2:D:7:DC:H5"	2:D:7:DC:H6	1.64	0.62
1:B:463:HIS:CD2	1:B:465:LEU:H	2.11	0.62
1:A:370:MET:HA	1:A:372:HIS:N	2.15	0.62
1:B:820:PHE:HB3	1:B:843:MET:HE2	1.83	0.61
1:A:239:ARG:HE	1:A:736:GLN:HE22	1.49	0.61
1:B:90:ASP:OD1	3:B:1008:HOH:O	2.16	0.61
1:A:264:GLN:HB2	2:C:10:DC:N4	2.15	0.60
1:A:149:ALA:HA	1:A:152:LYS:HE2	1.82	0.59
1:B:368:ARG:HH22	1:B:404:GLU:CD	2.06	0.59
1:A:239:ARG:HB2	2:C:9:DG:H3'	1.84	0.59
1:B:785:SER:O	1:B:786:ARG:NH1	2.36	0.58
1:A:141:GLU:HG3	1:A:144:LYS:NZ	2.18	0.58
1:B:201:SER:O	1:B:248:ARG:HD2	2.03	0.58
1:A:146:ARG:HA	1:A:146:ARG:HH11	1.68	0.58
1:A:65:LEU:O	1:A:69:LYS:HG3	2.03	0.58
1:A:684:ARG:HH12	1:A:813:VAL:C	2.07	0.57
1:A:575:GLU:HG2	1:A:611:LEU:HD23	1.84	0.57
1:A:97:PHE:HD1	1:A:629:MET:HE3	1.69	0.57
1:B:259:LEU:HD23	1:B:290:LEU:HD11	1.85	0.57
1:A:146:ARG:HH11	1:A:149:ALA:HB3	1.70	0.57
1:B:54:LEU:N	3:B:1024:HOH:O	2.38	0.57
1:B:447:THR:O	1:B:451:GLN:HG3	2.05	0.57
1:B:390:ARG:NH2	3:B:1023:HOH:O	2.38	0.56
1:B:239:ARG:HE	1:B:736:GLN:NE2	2.03	0.56
1:A:370:MET:HB3	1:A:373:GLU:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:DC:H5"	2:D:7:DC:C6	2.41	0.56
1:B:614:ARG:NH1	1:B:777:PRO:HG3	2.21	0.56
1:A:686:MET:HE1	1:A:700:THR:HA	1.87	0.56
1:A:678:ARG:HG3	1:A:721:PHE:HE2	1.70	0.55
1:A:684:ARG:NH1	1:A:813:VAL:O	2.30	0.55
1:A:269:MET:HE2	1:A:297:ILE:HG21	1.88	0.55
1:B:704:TYR:CZ	1:B:708:ARG:HD3	2.41	0.55
1:A:654:ASP:H	1:A:758:ASN:ND2	2.00	0.55
1:B:333:VAL:HG13	1:B:334:MET:O	2.06	0.55
1:B:142:ASN:O	1:B:146:ARG:HB2	2.07	0.55
1:B:672:PRO:HG2	1:B:675:LYS:HB2	1.89	0.55
1:A:91:ALA:HB2	1:A:902:TYR:HD1	1.72	0.54
1:A:175:VAL:HG12	1:A:312:THR:HG22	1.89	0.54
1:A:784:LYS:HB2	1:A:797:THR:H	1.73	0.54
1:B:765:PRO:HG2	1:B:927:GLU:HG3	1.89	0.54
1:B:144:LYS:N	3:B:1026:HOH:O	2.40	0.54
1:B:142:ASN:OD1	1:B:143:ALA:N	2.39	0.54
1:A:146:ARG:NH1	1:A:146:ARG:O	2.40	0.53
1:B:655:PRO:HA	1:B:698:HIS:CD2	2.43	0.53
1:A:141:GLU:C	1:A:145:LYS:NZ	2.59	0.53
1:A:871:LYS:NZ	3:A:1017:HOH:O	2.36	0.53
1:A:686:MET:CE	1:A:700:THR:HA	2.38	0.53
1:A:242:SER:O	1:A:243:ARG:NH1	2.42	0.53
1:A:183:THR:HG21	1:A:218:ILE:HD13	1.91	0.53
1:B:239:ARG:HB2	2:D:9:DG:H3'	1.91	0.53
1:B:164:GLN:OE1	1:B:167:ARG:NH2	2.41	0.52
1:A:738:SER:OG	1:A:752:CYS:HB3	2.08	0.52
1:B:177:SER:OG	3:B:1011:HOH:O	2.18	0.52
1:B:504:VAL:HG23	1:B:541:ALA:HB2	1.92	0.52
1:A:506:ASN:ND2	1:A:537:ARG:HH11	2.08	0.51
1:A:658:SER:OG	1:A:698:HIS:HD2	1.92	0.51
1:B:854:ASP:OD2	3:B:1012:HOH:O	2.19	0.51
1:A:506:ASN:ND2	1:A:508:GLY:H	2.08	0.51
1:B:324:ASN:ND2	3:B:1032:HOH:O	2.43	0.51
1:B:447:THR:HG23	1:B:450:GLY:N	2.23	0.51
1:A:513:THR:HG23	2:C:5:DC:C5	2.45	0.51
1:A:662:ALA:HB2	1:A:697:VAL:HG11	1.94	0.50
1:A:91:ALA:HB1	3:A:1071:HOH:O	2.11	0.50
1:A:353:PHE:O	1:A:354:GLN:HB2	2.12	0.50
1:A:913:LYS:NZ	3:A:1024:HOH:O	2.41	0.50
1:A:142:ASN:C	1:A:145:LYS:NZ	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:O	1:A:248:ARG:HD2	2.12	0.49
1:A:143:ALA:O	1:A:144:LYS:HB3	2.13	0.49
1:B:123:ASN:HD22	1:B:123:ASN:C	2.16	0.49
1:B:662:ALA:HB2	1:B:697:VAL:HG11	1.95	0.48
2:C:7:DC:H6	2:C:7:DC:H5"	1.77	0.48
1:A:285:VAL:HG23	1:A:568:GLU:CG	2.42	0.48
1:A:768:ARG:HD3	1:A:843:MET:O	2.13	0.48
1:A:684:ARG:NH2	3:A:1029:HOH:O	2.47	0.48
1:A:801:ASP:OD2	3:A:1012:HOH:O	2.20	0.48
1:A:264:GLN:HE21	2:C:10:DC:H41	1.61	0.47
1:A:107:GLU:O	1:A:111:GLU:HG3	2.15	0.47
1:A:268:LEU:HD23	1:A:300:HIS:HB2	1.96	0.47
1:B:658:SER:OG	1:B:698:HIS:HD2	1.97	0.47
1:B:147:LEU:HB2	3:B:1026:HOH:O	2.15	0.47
1:B:147:LEU:HD11	1:B:151:LYS:HE3	1.97	0.47
1:A:493:GLU:HG2	1:A:536:GLN:HG2	1.96	0.47
1:B:92:LYS:HE2	1:B:96:GLN:NE2	2.29	0.47
1:B:379:TYR:CZ	1:B:383:ILE:HD13	2.51	0.46
1:A:575:GLU:CG	1:A:611:LEU:HD23	2.45	0.46
1:B:381:ARG:O	1:B:384:ARG:NH1	2.48	0.46
1:B:183:THR:HG21	1:B:218:ILE:HD13	1.97	0.46
1:A:175:VAL:CG1	1:A:312:THR:HG22	2.45	0.46
1:B:129:ARG:NH2	3:B:1015:HOH:O	2.25	0.46
1:B:899:LYS:HA	1:B:899:LYS:HD2	1.76	0.46
1:A:784:LYS:HD3	1:A:785:SER:N	2.30	0.46
1:A:899:LYS:HA	1:A:899:LYS:HD2	1.75	0.46
1:A:154:PRO:HG2	1:A:180:CYS:HA	1.98	0.45
1:A:846:PRO:HB3	1:A:875:PHE:CZ	2.51	0.45
1:B:111:GLU:CB	1:B:115:ARG:HH12	2.30	0.45
1:B:793:ARG:HH22	1:B:815:SER:HG	1.60	0.45
1:A:784:LYS:HG3	1:A:785:SER:N	2.30	0.45
1:A:835:ASP:HB3	1:A:837:PHE:CZ	2.50	0.45
1:A:239:ARG:HE	1:A:736:GLN:NE2	2.14	0.45
1:A:493:GLU:HG2	1:A:536:GLN:CG	2.47	0.45
1:A:778:ASN:HB3	1:A:827:TYR:CZ	2.52	0.45
1:B:98:ARG:HE	1:B:102:SER:HB3	1.81	0.45
1:B:579:LEU:HG	1:B:632:ALA:HB2	1.99	0.45
1:B:148:GLU:OE1	1:B:151:LYS:HD2	2.16	0.45
1:A:698:HIS:HE1	3:A:1333:HOH:O	2.00	0.45
1:A:655:PRO:HA	1:A:698:HIS:CD2	2.53	0.44
1:A:642:LYS:O	1:A:646:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ARG:HA	1:A:879:ARG:HD2	1.89	0.44
1:A:205:ILE:HG12	1:A:274:VAL:HB	1.99	0.44
1:A:491:ILE:HB	2:C:6:DA:H5"	1.99	0.44
1:B:103:VAL:O	1:B:585:HIS:NE2	2.47	0.44
1:A:387:TYR:HB2	1:A:392:LEU:HD21	2.00	0.44
1:B:520:ASN:O	1:B:830:ARG:NH2	2.51	0.44
1:B:65:LEU:O	1:B:69:LYS:HG3	2.17	0.44
1:A:91:ALA:HB2	1:A:902:TYR:CD1	2.53	0.44
1:A:692:SER:HB2	1:A:842:THR:HG23	2.00	0.44
1:A:764:ILE:O	1:A:768:ARG:HG3	2.18	0.44
1:A:370:MET:HA	1:A:372:HIS:H	1.83	0.43
1:A:678:ARG:HG3	1:A:721:PHE:CE2	2.52	0.43
1:B:414:TYR:CZ	1:B:450:GLY:HA2	2.52	0.43
1:B:129:ARG:NH1	1:B:133:GLU:OE2	2.51	0.43
1:B:655:PRO:HA	1:B:698:HIS:CG	2.53	0.43
1:B:820:PHE:HB3	1:B:843:MET:CE	2.46	0.43
1:B:119:LEU:HD23	1:B:248:ARG:CZ	2.48	0.43
1:B:134:LEU:O	1:B:138:GLN:HG3	2.19	0.43
1:A:417:CYS:HB3	1:A:453:TRP:CZ3	2.54	0.43
1:B:239:ARG:NE	1:B:736:GLN:HE22	2.11	0.43
1:B:820:PHE:HD1	1:B:843:MET:CE	2.30	0.43
1:A:654:ASP:N	1:A:758:ASN:HD21	2.06	0.43
1:B:680:ASP:O	1:B:684:ARG:HG2	2.19	0.43
1:A:406:ILE:HD11	1:A:434:LYS:HD2	2.01	0.43
1:A:222:VAL:HG12	1:A:234:VAL:HG21	2.00	0.42
1:A:321:TYR:CD1	1:A:597:ILE:HG12	2.54	0.42
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.76	0.42
1:B:190:LEU:HD11	1:B:307:ILE:CD1	2.48	0.42
1:A:142:ASN:C	1:A:145:LYS:HZ3	2.21	0.42
1:B:569:ILE:HG12	1:B:600:PRO:HG3	2.00	0.42
1:B:112:THR:OG1	1:B:267:PRO:HD2	2.19	0.42
1:A:369:ARG:C	1:A:371:LYS:HB2	2.40	0.42
1:A:898:LYS:NZ	3:A:1015:HOH:O	2.36	0.42
1:B:856:VAL:HA	1:B:868:CYS:O	2.19	0.42
1:A:154:PRO:HA	1:A:157:LYS:HD3	2.02	0.42
1:A:579:LEU:HG	1:A:632:ALA:HB2	2.01	0.42
1:A:784:LYS:CG	1:A:785:SER:N	2.82	0.42
1:B:786:ARG:HA	1:B:786:ARG:HH11	1.85	0.42
1:A:111:GLU:O	1:A:115:ARG:HG3	2.19	0.42
1:B:157:LYS:HG3	3:B:1042:HOH:O	2.20	0.42
1:A:134:LEU:O	1:A:138:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:OE1	1:A:141:GLU:N	2.53	0.42
1:A:445:PRO:HA	3:A:1025:HOH:O	2.20	0.42
1:A:112:THR:OG1	1:A:267:PRO:HD2	2.20	0.41
1:A:239:ARG:HH21	1:A:736:GLN:NE2	2.17	0.41
1:A:264:GLN:HB2	2:C:10:DC:H41	1.82	0.41
1:A:399:GLU:CD	1:A:399:GLU:H	2.23	0.41
1:B:205:ILE:HG12	1:B:274:VAL:HB	2.02	0.41
1:B:314:ARG:HH11	1:B:314:ARG:HD2	1.67	0.41
1:A:908:GLU:O	1:A:913:LYS:HG2	2.21	0.41
1:B:93:PHE:CE2	1:B:630:HIS:CE1	3.09	0.41
1:B:820:PHE:HD1	1:B:843:MET:HE3	1.85	0.41
1:B:248:ARG:HD2	1:B:248:ARG:HH11	1.69	0.41
1:B:70:GLU:O	1:B:74:ASP:OD1	2.38	0.41
1:B:447:THR:CG2	3:B:1196:HOH:O	2.54	0.41
1:A:90:ASP:N	3:A:1040:HOH:O	2.54	0.41
1:A:665:PHE:CZ	1:A:666:LYS:HE2	2.56	0.41
1:B:239:ARG:HG2	1:B:240:LEU:HG	2.01	0.41
1:B:381:ARG:HD2	1:B:384:ARG:NH1	2.36	0.40
1:A:447:THR:O	1:A:451:GLN:HG3	2.20	0.40
1:A:793:ARG:HD2	2:C:2:DG:C6	2.56	0.40
1:A:861:THR:HG23	1:A:862:GLN:N	2.35	0.40
1:A:142:ASN:CA	1:A:145:LYS:NZ	2.70	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:GLN:NE2	1:B:603:GLU:OE1[1_565]	2.13	0.07
1:B:476:ARG:NH1	1:B:518:GLU:OE2[1_565]	2.16	0.04

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%)	820 (98%)	21 (2%)	0	100	100
1	B	843/944 (89%)	821 (97%)	22 (3%)	0	100	100
All	All	1684/1888 (89%)	1641 (97%)	43 (3%)	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	757/842 (90%)	749 (99%)	8 (1%)	73	85
1	B	759/842 (90%)	742 (98%)	17 (2%)	52	65
All	All	1516/1684 (90%)	1491 (98%)	25 (2%)	62	76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	94	GLN
1	A	137	ARG
1	A	272	LEU
1	A	290	LEU
1	A	573	LYS
1	A	805	ARG
1	A	862	GLN
1	B	58	VAL
1	B	94	GLN
1	B	114	GLU
1	B	123	ASN
1	B	137	ARG
1	B	146	ARG
1	B	301	ARG
1	B	314	ARG
1	B	347	SER
1	B	452	ARG

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Mol	Chain	Res	Type
1	B	454	ARG
1	B	476	ARG
1	B	540	ARG
1	B	640	MET
1	B	708	ARG
1	B	863	ASN
1	B	879	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	GLN
1	A	316	GLN
1	A	506	ASN
1	A	698	HIS
1	A	736	GLN
1	A	758	ASN
1	B	94	GLN
1	B	123	ASN
1	B	324	ASN
1	B	437	GLN
1	B	463	HIS
1	B	536	GLN
1	B	698	HIS
1	B	736	GLN

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 monosaccharides 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, 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%)	-0.35	9 (1%) 80 79	23, 41, 75, 108	0
1	B	851/944 (90%)	-0.39	8 (0%) 84 83	24, 39, 70, 97	0
2	C	9/9 (100%)	-0.50	0 100 100	37, 49, 60, 72	0
2	D	9/9 (100%)	-0.45	0 100 100	35, 48, 64, 81	0
All	All	1718/1906 (90%)	-0.37	17 (0%) 82 81	23, 40, 73, 108	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	795	ILE	4.9
1	A	785	SER	3.8
1	B	142	ASN	3.5
1	A	355	LYS	3.2
1	B	517	ILE	3.1
1	A	141	GLU	3.0
1	A	142	ASN	2.9
1	B	862	GLN	2.8
1	A	146	ARG	2.6
1	B	79	PRO	2.2
1	B	115	ARG	2.2
1	B	477	ARG	2.2
1	B	928	ARG	2.2
1	A	481	GLY	2.1
1	A	784	LYS	2.1
1	B	787	GLN	2.1
1	A	786	ARG	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 (i)

There are no monosaccharides 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.