



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:34 PM UTC

PDB ID : 5N9D / pdb_00005n9d
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 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

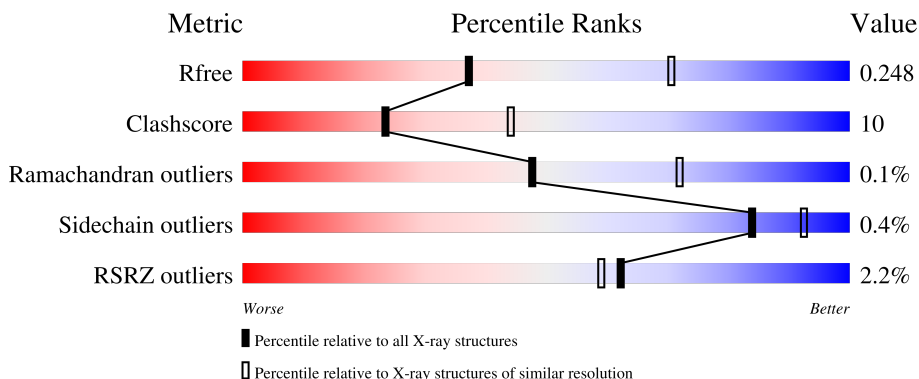
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	944	2% 69% 21% • 9%
1	B	944	2% 72% 19% • 8%
2	C	10	70% 30%
2	D	10	40% 60%

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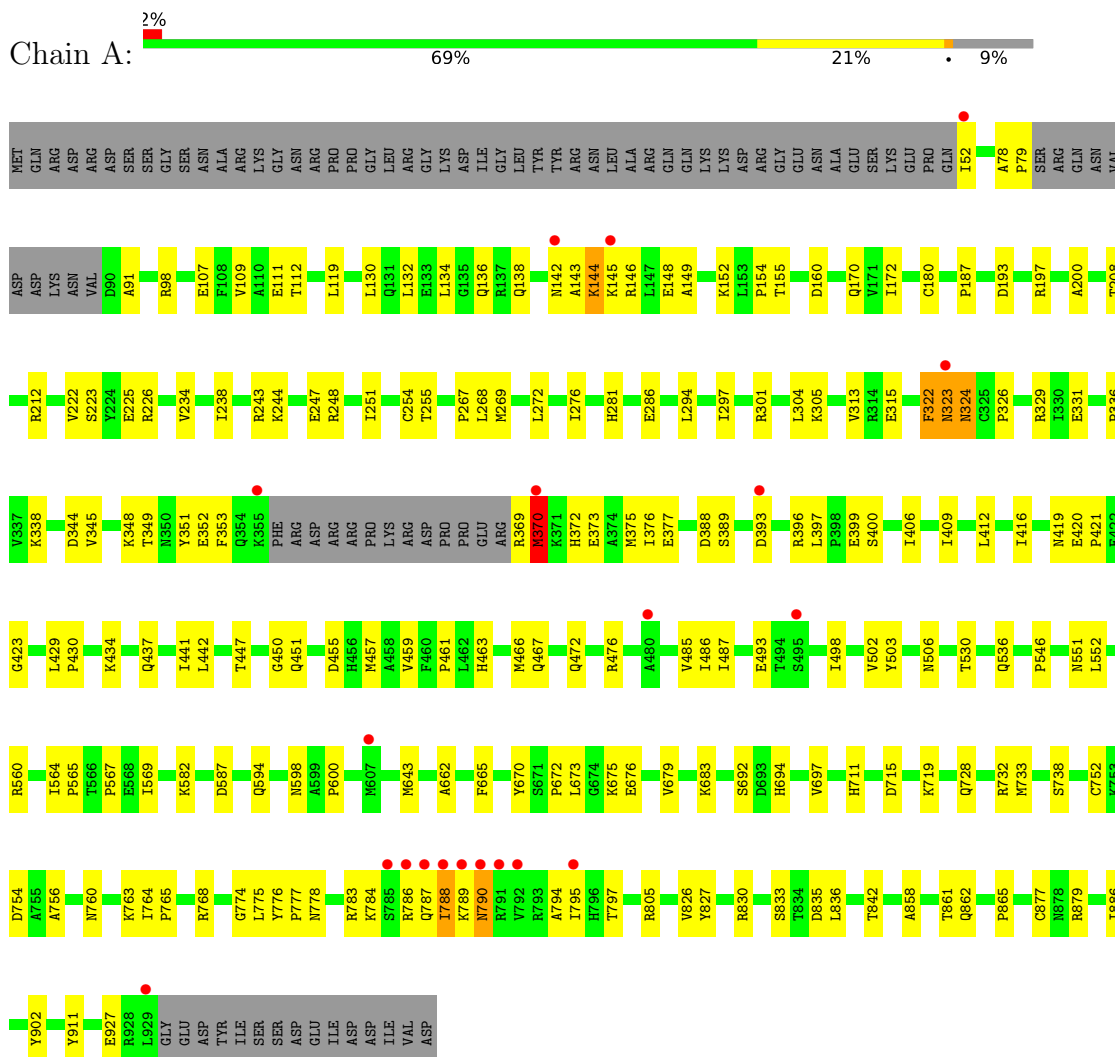
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	O	0	0
			2	2		

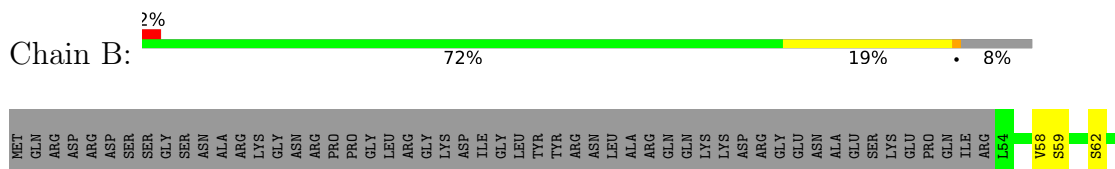
3 Residue-property plots [i](#)

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





4 Data and refinement statistics

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 56.68 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.7 (56.68-2.71) 98.7 (56.68-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.69Å)	Xtriage
Refinement program	PHENIX (dev_2427: ???)	Depositor
R, R_{free}	0.185 , 0.247 0.191 , 0.248	Depositor DCC
R_{free} test set	3103 reflections (4.83%)	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 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.42	0/6964	0.70	12/9398 (0.1%)
1	B	0.41	0/7027	0.69	6/9490 (0.1%)
2	C	0.41	0/239	0.57	0/369
2	D	0.54	0/239	0.64	0/369
All	All	0.42	0/14469	0.69	18/19626 (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 (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	PRO	N-CA-CB	9.46	113.19	103.25
1	A	322	PHE	CA-C-N	7.58	138.35	125.02
1	A	322	PHE	C-N-CA	7.58	138.35	125.02
1	A	323	ASN	N-CA-C	7.57	125.22	113.72
1	B	360	ARG	CA-C-N	6.38	127.81	119.84
1	B	360	ARG	C-N-CA	6.38	127.81	119.84
1	A	323	ASN	N-CA-CB	-6.16	104.59	113.65
1	A	789	LYS	CA-C-N	-6.16	111.65	120.89
1	A	789	LYS	C-N-CA	-6.16	111.65	120.89
1	B	363	ARG	N-CA-C	-5.97	101.34	110.30
1	A	324	ASN	CA-C-O	-5.73	115.24	121.20
1	A	861	THR	CA-C-N	-5.60	111.81	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	861	THR	C-N-CA	-5.60	111.81	120.88
1	A	790	ASN	N-CA-C	5.19	119.08	111.04
1	A	370	MET	CA-C-N	5.17	131.00	121.70
1	A	370	MET	C-N-CA	5.17	131.00	121.70
1	B	664	SER	CA-C-N	5.06	131.02	122.12
1	B	664	SER	C-N-CA	5.06	131.02	122.12

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	157	0
1	B	6904	0	6948	126	0
2	C	213	0	114	3	0
2	D	213	0	114	8	0
3	A	54	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	289	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 (289) 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: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:B:779:MET:HE3	1:B:849:LEU:HD13	1.64	0.78
1:A:149:ALA:HA	1:A:152:LYS:HE3	1.66	0.78
1:A:461:PRO:HB2	1:A:466:MET:HE1	1.66	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:OE1	1:A:399:GLU:N	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:H	1:A:673:LEU:HD12	1.62	0.63
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:OE1	1:B:399:GLU:N	2.21	0.61
1:B:121:TRP:O	1:B:248:ARG:NH2	2.34	0.61
1:A:463:HIS:HB2	1:A:466:MET:HE2	1.83	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:A:461:PRO:HB2	1:A:466:MET:CE	2.31	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:675:LYS:HZ3	1:B:678:ARG:HD3	1.69	0.57
1:B:692:SER:HB2	1:B:842:THR:HG23	1.86	0.57
1:A:665:PHE:HB2	1:A:733:MET:HE1	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:OE1	1:A:286:GLU:N	2.35	0.56
1:A:132:LEU:O	1:A:136:GLN:HG3	2.05	0.56
1:A:506:ASN:HB3	1:A:551:ASN:ND2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ARG:HB3	1:A:794:ALA:HA	1.86	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:134:LEU:C	1:A:138:GLN:HE21	2.15	0.54
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
1:A:247:GLU:OE2	3:A:1004:HOH:O	2.18	0.54
1:A:463:HIS:CB	1:A:466:MET:HE2	2.37	0.54
1:A:694:HIS:ND1	1:A:842:THR:OG1	2.41	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:B:144:LYS:C	1:B:145:LYS:HD2	2.34	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
1:B:174:ILE:HD12	1:B:309:MET:HE2	1.91	0.53
1:A:269:MET:HE2	1:A:297:ILE:HG21	1.91	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:360:ARG:C	1:B:362:LYS:H	2.20	0.50
1:A:269:MET:HE1	1:A:294:LEU:CD2	2.42	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:B:442:LEU:HB3	1:B:457:MET:HE1	1.93	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
1:A:760:ASN:CG	1:A:763:LYS:NZ	2.69	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:A:145:LYS:HE2	1:A:148:GLU:CD	2.38	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:442:LEU:HD22	1:A:457:MET:HE1	1.95	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:79:PRO:O	3:A:1005:HOH:O	2.20	0.48
1:A:369:ARG:NE	1:A:369:ARG:HA	2.29	0.48
1:A:643:MET:HE3	1:A:774:GLY:HA3	1.95	0.48
1:A:594:GLN:NE2	3:A:1008:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:143:ALA:C	1:A:145:LYS:H	2.21	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:HA	1:A:146:ARG:HH11	1.80	0.47
1:B:145:LYS:HD2	1:B:145:LYS:N	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: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
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: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: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:78:ALA:HB2	1:A:911:TYR:CG	2.52	0.45
1:A:344:ASP:O	1:A:348:LYS:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLU:CD	1:A:396:ARG:HH21	2.24	0.45
1:B:832:LYS:HB2	1:B:836:LEU:HD13	1.99	0.45
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:272:LEU:C	1:B:272:LEU:HD12	2.42	0.44
1:B:430:PRO:HA	1:B:510:THR:HA	1.99	0.44
1:A:530:THR:HG21	1:A:564:ILE:C	2.42	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: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: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:691:ARG:HH12	1:B:819:GLY:C	2.25	0.43
1:B:850:ILE:O	1:B:889:ARG:HD2	2.18	0.43
1:B:696:MET:HE2	1:B:813:VAL:CG1	2.49	0.43
1:B:144:LYS:O	1:B:145:LYS:HD2	2.18	0.42
1:B:186:VAL:HB	1:B:309:MET:HE1	2.01	0.42
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:B:331:GLU:H	1:B:331:GLU:CD	2.26	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:784:LYS:HB2	1:A:797:THR:N	2.34	0.42
1:A:786:ARG:HD2	1:A:788:ILE:N	2.20	0.42
1:B:206:ILE:HD13	1:B:252:THR:HB	2.01	0.42
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.83	0.42
1:B:722:LEU:HA	1:B:722:LEU:HD23	1.81	0.42
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.85	0.42
1:A:154:PRO:HB3	1:A:331:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HG22	1:A:255:THR:HG23	2.02	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:244:LYS:NZ	2:C:11:DT:H5"	2.35	0.42
1:A:269:MET:HB3	1:A:272:LEU:HD21	2.01	0.42
1:A:457:MET:HE3	1:A:457:MET:HB2	1.89	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:352:GLU:CD	1:A:353:PHE:H	2.28	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:155:THR:OG1	1:A:180:CYS:O	2.26	0.41
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.86	0.41
1:B:155:THR:OG1	1:B:180:CYS:O	2.18	0.41
1:B:696:MET:HE2	1:B:813:VAL:HG13	2.02	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
1:B:558:GLU:HA	1:B:561:MET:HE2	2.02	0.41
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:399:GLU:N	1:A:399:GLU:CD	2.79	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:58:VAL:HG13	1:B:847:MET:HE2	2.03	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%)	43	66
All	All	1711/1888 (91%)	1677 (98%)	32 (2%)	2 (0%)	48	72

All (2) Ramachandran outliers are listed below:

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

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%)	755 (100%)	2 (0%)	86	93
1	B	759/842 (90%)	755 (100%)	4 (0%)	81	91
All	All	1516/1684 (90%)	1510 (100%)	6 (0%)	84	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	A	886	ILE
1	B	59	SER
1	B	147	LEU
1	B	223	SER
1	B	607	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	96	GLN
1	A	136	GLN
1	A	138	GLN
1	A	164	GLN
1	A	169	ASN
1	A	514	ASN
1	A	551	ASN
1	A	594	GLN
1	A	598	ASN
1	A	620	GLN
1	A	711	HIS
1	B	94	GLN
1	B	116	ASN
1	B	123	ASN
1	B	138	GLN

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Mol	Chain	Res	Type
1	B	164	GLN
1	B	185	GLN
1	B	232	ASN
1	B	237	GLN
1	B	270	HIS
1	B	467	GLN
1	B	506	ASN
1	B	630	HIS
1	B	736	GLN
1	B	743	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	855/944 (90%)	-0.02	20 (2%) 61 58	28, 57, 106, 133	0
1	B	866/944 (91%)	-0.08	18 (2%) 63 60	29, 54, 95, 136	0
2	C	10/10 (100%)	-0.02	0 100 100	52, 76, 94, 100	0
2	D	10/10 (100%)	0.09	0 100 100	45, 65, 79, 90	0
All	All	1741/1908 (91%)	-0.05	38 (2%) 62 59	28, 55, 101, 136	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	790	ASN	4.9
1	A	791	ARG	4.3
1	B	790	ASN	4.2
1	A	792	VAL	4.2
1	B	361	PRO	3.7
1	A	355	LYS	3.5
1	A	788	ILE	3.5
1	B	791	ARG	3.2
1	B	356	PHE	3.2
1	B	929	LEU	2.8
1	A	786	ARG	2.8
1	A	795	ILE	2.7
1	A	929	LEU	2.7
1	B	366	PRO	2.6
1	A	789	LYS	2.6
1	B	149	ALA	2.5
1	B	357	ARG	2.5
1	B	359	ARG	2.4
1	A	480	ALA	2.4
1	A	495	SER	2.3
1	A	785	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	787	GLN	2.3
1	B	792	VAL	2.3
1	B	481	GLY	2.2
1	B	145	LYS	2.2
1	A	370	MET	2.2
1	B	143	ALA	2.2
1	A	142	ASN	2.2
1	B	364	ASP	2.2
1	A	607	MET	2.2
1	A	145	LYS	2.1
1	B	354	GLN	2.1
1	A	52	ILE	2.1
1	B	788	ILE	2.1
1	A	323	ASN	2.1
1	B	675	LYS	2.0
1	A	393	ASP	2.0
1	B	862	GLN	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 oligosaccharides 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.