



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:55 AM UTC

PDB ID : 5N8R / pdb_00005n8r
Title : Crystal Structure of Drosophila 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 : 4-5-2 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

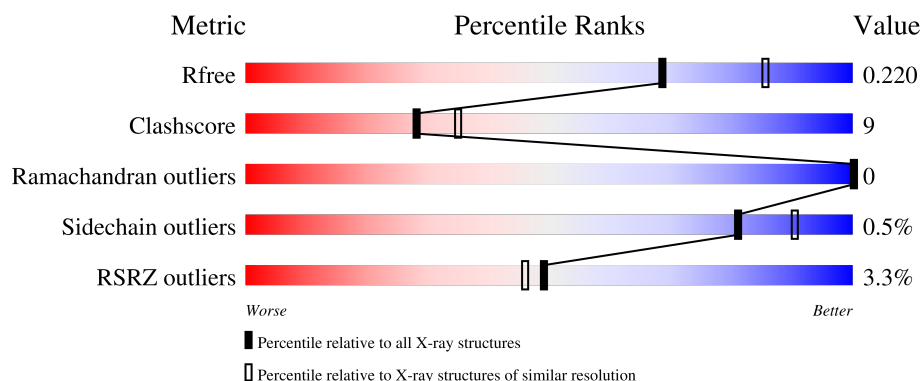
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	3% 73% 16% 10%
1	B	944	3% 75% 15% 10%
2	C	9	33% 67%
2	D	9	44% 56%

2 Entry composition

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:

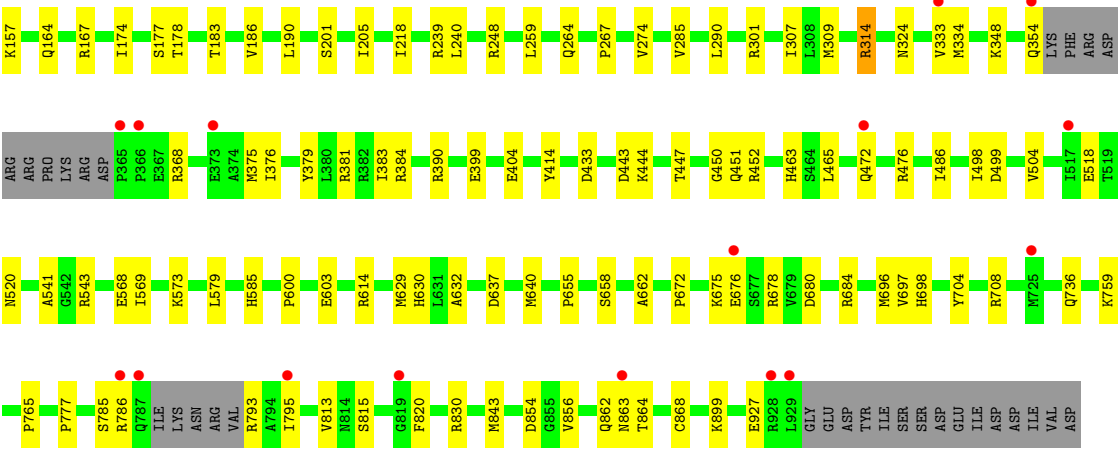
Chain	Residue	Modelled	Actual	Comment	Reference
A	943	VAL	-	expression tag	UNP Q8SWT2
A	944	ASP	-	expression tag	UNP Q8SWT2
B	943	VAL	-	expression tag	UNP Q8SWT2
B	944	ASP	-	expression tag	UNP Q8SWT2

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*AP*GP*CP*AP*CP*TP*GP*C)-3').

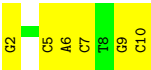
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			185	87	36	53	9			
2	D	9	Total	C	N	O	P	0	0	0
			185	87	36	53	9			

- 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		



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



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



4 Data and refinement statistics

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 – 2.20 149.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (149.90-2.20) 99.3 (149.90-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.176 , 0.219 0.179 , 0.220	Depositor DCC
R_{free} test set	5865 reflections (4.97%)	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)	0.35 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.*

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	0.43	3/6933 (0.0%)	0.70	13/9353 (0.1%)
1	B	0.41	0/6950	0.65	2/9378 (0.0%)
2	C	0.51	0/207	0.56	0/317
2	D	0.56	0/207	0.63	0/317
All	All	0.42	3/14297 (0.0%)	0.67	15/19365 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	684	ARG	CD-NE	-7.37	1.35	1.46
1	A	145	LYS	CD-CE	-6.48	1.33	1.52
1	A	684	ARG	CZ-NH2	5.12	1.40	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	LYS	CD-CE-NZ	-7.25	88.69	111.90
1	A	880	GLU	N-CA-CB	-6.84	100.06	110.12
1	A	684	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	A	571	ARG	CG-CD-NE	6.21	125.67	112.00
1	A	141	GLU	CA-C-N	5.45	131.95	121.54
1	A	141	GLU	C-N-CA	5.45	131.95	121.54
1	A	880	GLU	CB-CG-CD	-5.42	103.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	880	GLU	CA-CB-CG	5.40	124.91	114.10
1	A	535	GLN	CB-CA-C	5.40	119.75	110.79
1	B	115	ARG	CD-NE-CZ	5.34	131.87	124.40
1	B	115	ARG	CB-CG-CD	5.17	123.18	111.30
1	A	145	LYS	CA-CB-CG	5.16	124.41	114.10
1	A	684	ARG	CB-CA-C	-5.10	102.32	110.79
1	A	879	ARG	CA-C-N	5.05	127.05	120.28
1	A	879	ARG	C-N-CA	5.05	127.05	120.28

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	138	0
1	B	6829	0	6918	107	2
2	C	185	0	101	8	0
2	D	185	0	101	7	0
3	A	377	0	0	19	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	250	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 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)
1:A:142:ASN:N	1:A:145:LYS:HZ1	1.53	1.06
1:A:784:LYS:HG2	1:A:796:HIS:HA	1.38	1.05
1:A:666:LYS:NZ	3:A:1003:HOH:O	1.92	1.02
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:A:686:MET:HE3	1:A:700:THR:HA	1.55	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:HZ1	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: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:B:862:GLN:CD	1:B:863:ASN:H	1.90	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:573:LYS:NZ	3:B:1005:HOH:O	2.11	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: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:269:MET:HE1	1:A:294:LEU:CD2	2.22	0.70
1:B:820:PHE:HB3	1:B:843:MET:HE2	1.74	0.69
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:A:141:GLU:C	1:A:145:LYS:HZ1	2.02	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HZ2	1.60	0.66
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:368:ARG:HH22	1:B:404:GLU:CD	2.06	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:B:486:ILE:HD13	1:B:498:ILE:HD13	1.81	0.62
1:A:684:ARG:HH12	1:A:813:VAL:C	2.07	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:269:MET:HE1	1:A:294:LEU:HD21	1.81	0.62
1:A:370:MET:HA	1:A:372:HIS:N	2.15	0.62
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:470:GLU:OE1	1:A:670:TYR:OH	2.16	0.61
1:B:348:LYS:NZ	3:B:1004:HOH:O	2.09	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:93:PHE:CE2	1:B:629:MET:HE2	2.37	0.59
1:A:239:ARG:HB2	2:C:9:DG:H3'	1.84	0.59
1:A:871:LYS:NZ	3:A:1017:HOH:O	2.36	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:A:178:THR:HG22	1:A:334:MET:HE3	1.85	0.58
1:B:201:SER:O	1:B:248:ARG:HD2	2.03	0.58
1:A:141:GLU:C	1:A:145:LYS:NZ	2.59	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:B:696:MET:HE2	1:B:813:VAL:HG13	1.85	0.58
1:A:575:GLU:HG2	1:A:611:LEU:HD23	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:269:MET:HE2	1:A:297:ILE:HD13	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:142:ASN:C	1:A:145:LYS:NZ	2.66	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:123:ASN:HD22	1:B:123:ASN:C	2.16	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: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:B:178:THR:HG22	1:B:334:MET:HE2	1.91	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:269:MET:HE1	1:A:294:LEU:HD23	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:141:GLU:HG3	1:A:144:LYS:HZ1	1.78	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:A:142:ASN:C	1:A:145:LYS:HZ1	2.21	0.47
1:A:333:VAL:O	1:A:334:MET:HE2	2.15	0.47
1:B:147:LEU:HB2	3:B:1026:HOH:O	2.15	0.47
1:A:369:ARG:C	1:A:371:LYS:HB2	2.40	0.47
1:B:147:LEU:HD11	1:B:151:LYS:HE3	1.97	0.47
1:A:913:LYS:NZ	3:A:1024:HOH:O	2.41	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:A:637:ASP:HB2	1:A:640:MET:HE2	1.98	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:A:399:GLU:CD	1:A:399:GLU:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:97:PHE:HD1	1:A:629:MET:HE3	1.82	0.45
1:A:784:LYS:HG3	1:A:785:SER:N	2.30	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:186:VAL:HB	1:A:309:MET:HE1	1.99	0.44
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
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:B:399:GLU:CD	1:B:399:GLU:H	2.26	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:186:VAL:HB	1:B:309:MET:HE1	1.99	0.43
1:B:414:TYR:CZ	1:B:450:GLY:HA2	2.52	0.43
1:A:186:VAL:CB	1:A:309:MET:HE1	2.48	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:B:676:GLU:H	1:B:676:GLU:CD	2.26	0.43
1:B:696:MET:HE2	1:B:813:VAL:CG1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:174:ILE:HD12	1:B:309:MET:HE2	2.01	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:A:530:THR:HG21	1:A:564:ILE:C	2.44	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
1:A:665:PHE:HB2	1:A:733:MET:HE1	2.01	0.42
1:B:375:MET:HE2	1:B:376:ILE:HB	2.01	0.42
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:847:MET:HE2	1:A:847:MET:HB2	1.98	0.42
1:B:452:ARG:HD3	1:B:452:ARG:C	2.45	0.41
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: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: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:B:820:PHE:HD1	1:B:843:MET:HE3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:443:ASP:OD2	1:B:444:LYS:NZ	2.49	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%)	754 (100%)	3 (0%)	84	92
1	B	759/842 (90%)	754 (99%)	5 (1%)	76	87
All	All	1516/1684 (90%)	1508 (100%)	8 (0%)	81	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	272	LEU
1	A	880	GLU
1	B	58	VAL
1	B	123	ASN
1	B	301	ARG
1	B	314	ARG
1	B	640	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	232	ASN
1	A	261	GLN
1	A	264	GLN
1	A	300	HIS
1	A	316	GLN
1	A	506	ASN
1	A	522	GLN
1	A	698	HIS
1	A	735	ASN
1	A	736	GLN
1	A	758	ASN
1	A	781	HIS
1	A	831	GLN
1	B	94	GLN
1	B	95	GLN
1	B	123	ASN
1	B	169	ASN
1	B	237	GLN
1	B	300	HIS
1	B	324	ASN
1	B	437	GLN

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Mol	Chain	Res	Type
1	B	463	HIS
1	B	467	GLN
1	B	536	GLN
1	B	698	HIS
1	B	699	ASN
1	B	720	ASN
1	B	736	GLN
1	B	781	HIS
1	B	787	GLN
1	B	863	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	849/944 (89%)	-0.02	27 (3%)	50	47	23, 41, 75, 108	0
1	B	851/944 (90%)	-0.08	29 (3%)	48	45	24, 39, 70, 97	0
2	C	9/9 (100%)	-0.24	0	100	100	37, 49, 60, 72	0
2	D	9/9 (100%)	-0.20	0	100	100	35, 48, 64, 81	0
All	All	1718/1906 (90%)	-0.05	56 (3%)	49	46	23, 40, 73, 108	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	LYS	5.1
1	A	929	LEU	5.1
1	B	79	PRO	4.6
1	B	517	ILE	4.5
1	A	813	VAL	4.4
1	A	79	PRO	4.3
1	B	365	PRO	4.2
1	A	795	ILE	3.6
1	B	929	LEU	3.6
1	A	785	SER	3.5
1	B	115	ARG	3.5
1	B	78	ALA	3.5
1	A	334	MET	3.5
1	B	366	PRO	3.4
1	A	142	ASN	3.4
1	A	146	ARG	3.3
1	B	91	ALA	3.2
1	A	91	ALA	3.2
1	A	481	GLY	3.1
1	B	90	ASP	3.1
1	A	370	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	795	ILE	2.9
1	A	571	ARG	2.9
1	B	928	ARG	2.9
1	B	142	ASN	2.9
1	B	139	LEU	2.8
1	A	354	GLN	2.8
1	A	371	LYS	2.8
1	A	141	GLU	2.7
1	B	354	GLN	2.7
1	B	143	ALA	2.6
1	A	178	THR	2.6
1	A	684	ARG	2.6
1	A	90	ASP	2.6
1	B	137	ARG	2.5
1	B	140	GLU	2.5
1	A	324	ASN	2.5
1	A	143	ALA	2.5
1	B	787	GLN	2.4
1	B	98	ARG	2.4
1	A	369	ARG	2.3
1	A	784	LYS	2.3
1	A	861	THR	2.3
1	B	373	GLU	2.3
1	A	144	LYS	2.3
1	B	141	GLU	2.2
1	B	725	MET	2.1
1	B	472	GLN	2.1
1	A	145	LYS	2.1
1	B	863	ASN	2.1
1	B	786	ARG	2.1
1	B	676	GLU	2.1
1	B	819	GLY	2.1
1	A	796	HIS	2.1
1	B	138	GLN	2.0
1	B	333	VAL	2.0

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 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.