



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:48 AM UTC

PDB ID : 2Y9Y / pdb_00002y9y
Title : Chromatin Remodeling Factor ISW1a(del_ATPase)
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mele, K.; Sargent, D.F.; Richmond, T.J.
Deposited on : 2011-02-17
Resolution : 3.25 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

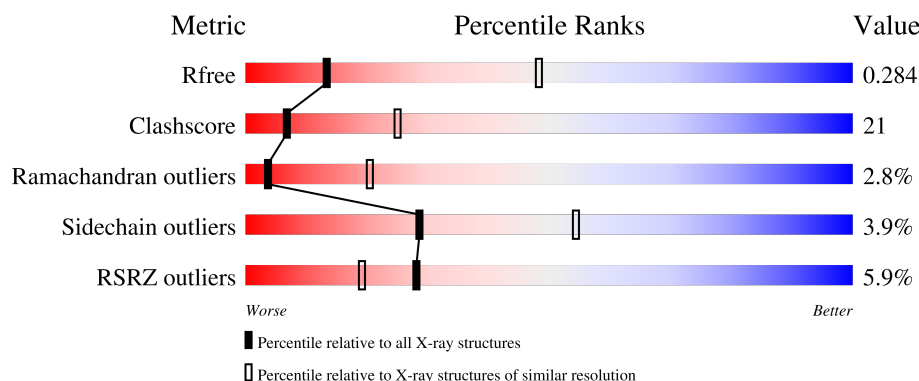
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	374	5% 46% 26% • 26%
2	B	624	5% 54% 37% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7170 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 IMITATION SWITCH PROTEIN 1 (DEL_ATPASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2317	1473	399	437	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	MET	-	expression tag	UNP P38144
A	815	GLN	LYS	engineered mutation	UNP P38144
A	844	LYS	ASP	engineered mutation	UNP P38144
A	848	GLN	GLU	engineered mutation	UNP P38144
A	851	GLN	LYS	engineered mutation	UNP P38144
A	853	GLU	GLN	engineered mutation	UNP P38144
A	1130	HIS	-	expression tag	UNP P38144
A	1131	HIS	-	expression tag	UNP P38144
A	1132	HIS	-	expression tag	UNP P38144
A	1133	HIS	-	expression tag	UNP P38144
A	1134	HIS	-	expression tag	UNP P38144
A	1135	HIS	-	expression tag	UNP P38144

- Molecule 2 is a protein called ISWI ONE COMPLEX PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	592	Total	C	N	O	S	0	0	0
			4853	3123	818	897	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	126	MET	-	expression tag	UNP P43596
B	682	LYS	ASN	engineered mutation	UNP P43596



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	206.97Å 206.97Å 215.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.87 – 3.25 29.87 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.87-3.25) 99.8 (29.87-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 3.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.283 , 0.296 0.279 , 0.284	Depositor DCC
R_{free} test set	1381 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	120.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/2368	0.70	0/3186
2	B	0.25	0/4974	0.66	0/6723
All	All	0.25	0/7342	0.67	0/9909

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2317	0	2300	98	0
2	B	4853	0	4857	213	0
All	All	7170	0	7157	307	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 21.

All (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:LYS:HB2	2:B:328:PRO:HD3	1.50	0.91
1:A:918:LYS:HB2	1:A:922:GLU:HG3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:LYS:HA	2:B:296:SER:HB3	1.54	0.87
2:B:339:THR:HB	2:B:340:PRO:HD3	1.61	0.83
2:B:413:LEU:HD22	2:B:533:LEU:HB2	1.58	0.83
1:A:937:ILE:HG21	1:A:940:TYR:HB3	1.60	0.82
2:B:690:LEU:HB3	2:B:691:PRO:HD3	1.60	0.82
2:B:152:PRO:HG3	2:B:431:ARG:HD2	1.62	0.80
2:B:237:LEU:H	2:B:237:LEU:HD23	1.46	0.79
2:B:164:VAL:HG22	2:B:609:PRO:HB2	1.61	0.79
2:B:212:LEU:HD11	2:B:254:MET:HE2	1.66	0.78
2:B:153:LEU:H	2:B:153:LEU:HD23	1.50	0.77
2:B:381:LEU:HD12	2:B:381:LEU:H	1.51	0.76
2:B:554:LEU:H	2:B:598:SER:HB2	1.51	0.76
2:B:255:ASN:HD21	2:B:380:ILE:H	1.34	0.75
1:A:805:HIS:CD2	1:A:806:SER:H	2.04	0.75
2:B:324:ASP:HA	2:B:330:THR:HG21	1.68	0.74
2:B:373:ARG:H	2:B:373:ARG:HD3	1.51	0.74
2:B:144:PRO:HB2	2:B:421:VAL:HG21	1.68	0.73
2:B:150:VAL:HB	2:B:525:PRO:HG3	1.71	0.73
2:B:260:SER:HA	2:B:282:THR:HG21	1.72	0.71
1:A:974:PRO:O	1:A:998:ARG:HD2	1.92	0.70
1:A:805:HIS:CG	1:A:806:SER:H	2.09	0.70
2:B:316:ARG:HD2	2:B:360:ASN:HB3	1.71	0.70
2:B:167:ARG:H	2:B:167:ARG:HD3	1.56	0.70
2:B:149:SER:HB2	2:B:519:ASP:HB3	1.73	0.70
1:A:905:ASN:HD21	2:B:343:ASP:HB3	1.55	0.69
1:A:993:SER:HB3	1:A:996:GLU:HG3	1.75	0.69
2:B:509:TRP:HB3	2:B:513:PHE:HE2	1.58	0.69
2:B:150:VAL:HG12	2:B:431:ARG:H	1.58	0.69
1:A:983:PRO:HA	1:A:1052:CYS:HB3	1.76	0.67
1:A:934:ILE:O	1:A:937:ILE:HG12	1.93	0.67
1:A:1041:GLU:HG2	1:A:1044:ARG:HH21	1.60	0.66
2:B:393:ARG:O	2:B:396:THR:HG22	1.96	0.66
1:A:915:ALA:N	1:A:916:PRO:HD3	2.11	0.66
2:B:150:VAL:HA	2:B:431:ARG:HB2	1.76	0.66
2:B:228:LYS:HE3	2:B:228:LYS:HA	1.77	0.66
2:B:255:ASN:HB3	2:B:287:LEU:HD11	1.77	0.65
1:A:1003:MET:SD	1:A:1021:GLU:HG2	2.37	0.65
1:A:967:LYS:HD3	1:A:1057:PHE:CE2	2.32	0.64
2:B:451:ILE:HD12	2:B:512:LEU:HD22	1.79	0.64
2:B:426:THR:HG23	2:B:427:GLN:HG3	1.80	0.63
2:B:586:ALA:HA	2:B:589:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:PRO:HB3	1:A:879:TRP:CE3	2.34	0.62
2:B:403:SER:HB3	2:B:406:ILE:HG12	1.82	0.62
2:B:358:ASN:HD22	2:B:358:ASN:H	1.47	0.62
1:A:811:PRO:HB3	1:A:879:TRP:HE3	1.65	0.61
2:B:315:TRP:O	2:B:363:LEU:HB2	2.00	0.61
2:B:641:LEU:HD21	2:B:710:LEU:HB2	1.80	0.61
2:B:341:VAL:HG22	2:B:343:ASP:H	1.65	0.61
1:A:814:LEU:HD23	1:A:817:LEU:HD12	1.82	0.60
2:B:353:ASN:HD22	2:B:353:ASN:N	2.00	0.60
2:B:557:TYR:HA	2:B:561:LEU:HD11	1.82	0.60
1:A:875:MET:HB3	1:A:879:TRP:HE1	1.66	0.60
2:B:159:LYS:NZ	2:B:159:LYS:HB3	2.15	0.60
1:A:974:PRO:HB2	1:A:1002:LEU:HD21	1.82	0.60
1:A:914:LEU:HD12	1:A:915:ALA:H	1.67	0.59
2:B:256:LEU:HD22	2:B:284:TRP:CD1	2.37	0.59
2:B:475:ASP:O	2:B:479:LYS:HG3	2.03	0.59
1:A:1006:LYS:HA	1:A:1006:LYS:HE3	1.85	0.58
2:B:578:LYS:HD3	2:B:584:TYR:CE1	2.38	0.58
2:B:556:SER:HA	2:B:566:PHE:CD2	2.39	0.58
2:B:697:ASN:HA	2:B:700:ARG:NE	2.19	0.58
1:A:807:HIS:CG	1:A:807:HIS:O	2.57	0.57
1:A:914:LEU:CD1	1:A:915:ALA:H	2.17	0.57
2:B:150:VAL:O	2:B:430:PRO:HA	2.04	0.57
1:A:967:LYS:HD3	1:A:1057:PHE:HE2	1.68	0.57
2:B:358:ASN:H	2:B:358:ASN:ND2	2.01	0.57
2:B:384:LYS:O	2:B:388:ARG:HG3	2.03	0.57
2:B:661:LYS:HA	2:B:661:LYS:HE2	1.86	0.57
2:B:261:LEU:O	2:B:265:THR:HG22	2.05	0.57
1:A:888:ASN:HB2	1:A:891:GLU:HG3	1.86	0.57
2:B:151:ILE:HD11	2:B:525:PRO:HB3	1.87	0.56
2:B:510:VAL:HB	2:B:511:PRO:HD3	1.87	0.56
2:B:458:ARG:HB2	2:B:461:LYS:HB3	1.87	0.56
2:B:516:GLU:HB3	2:B:517:LEU:HD12	1.87	0.56
2:B:400:ALA:HA	2:B:406:ILE:HD11	1.87	0.56
2:B:454:ARG:HH21	2:B:516:GLU:HG3	1.70	0.56
2:B:411:TYR:HA	2:B:414:THR:HG22	1.88	0.55
2:B:193:SER:HB2	2:B:201:GLN:NE2	2.20	0.55
1:A:875:MET:HB3	1:A:879:TRP:NE1	2.22	0.55
2:B:407:HIS:O	2:B:410:ILE:HG13	2.07	0.55
2:B:321:SER:C	2:B:323:GLN:H	2.15	0.55
2:B:476:LEU:HA	2:B:479:LYS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:PRO:CA	1:A:1052:CYS:HB3	2.36	0.54
1:A:961:GLN:HE21	1:A:1009:LEU:HG	1.72	0.54
2:B:152:PRO:HD2	2:B:429:VAL:O	2.07	0.54
2:B:630:LEU:HD13	2:B:640:PHE:CZ	2.41	0.54
2:B:153:LEU:H	2:B:153:LEU:CD2	2.20	0.54
1:A:800:LYS:HB3	1:A:822:ARG:HE	1.73	0.54
1:A:987:ASN:N	1:A:987:ASN:HD22	2.05	0.54
2:B:245:LYS:O	2:B:245:LYS:HD3	2.08	0.54
2:B:447:LEU:HD22	2:B:513:PHE:HE1	1.71	0.54
1:A:1011:ARG:HG3	1:A:1012:ASP:OD1	2.08	0.54
1:A:937:ILE:HD13	1:A:940:TYR:HB3	1.90	0.54
2:B:186:MET:HE1	2:B:205:PHE:HD2	1.74	0.53
2:B:732:PRO:HB3	2:B:737:LEU:HD13	1.90	0.53
2:B:739:ARG:NH1	2:B:739:ARG:HB2	2.23	0.53
1:A:833:PRO:HG2	1:A:858:LEU:HA	1.90	0.53
2:B:277:LYS:HE3	2:B:277:LYS:HA	1.91	0.53
2:B:537:GLU:CD	2:B:537:GLU:H	2.17	0.53
1:A:866:GLN:HG3	1:A:867:PRO:HD2	1.91	0.53
2:B:473:LYS:N	2:B:474:PRO:CD	2.71	0.53
1:A:807:HIS:CD2	1:A:938:GLU:H	2.27	0.52
2:B:467:GLN:HE22	2:B:469:LYS:HB2	1.74	0.52
1:A:914:LEU:HB2	1:A:916:PRO:HG3	1.92	0.52
2:B:524:ASN:HB3	2:B:527:SER:OG	2.10	0.52
2:B:608:THR:OG1	2:B:609:PRO:HD3	2.09	0.52
2:B:537:GLU:C	2:B:539:PHE:H	2.18	0.52
2:B:140:PRO:HB3	2:B:457:ILE:HG12	1.91	0.52
2:B:212:LEU:HD12	2:B:254:MET:HG3	1.92	0.52
2:B:271:ASP:HB3	2:B:273:LYS:HE3	1.91	0.52
2:B:149:SER:HB2	2:B:519:ASP:CB	2.40	0.52
2:B:150:VAL:HG22	2:B:521:PRO:HA	1.92	0.52
2:B:167:ARG:H	2:B:167:ARG:CD	2.20	0.52
2:B:186:MET:HE1	2:B:552:PRO:HB3	1.92	0.52
1:A:838:VAL:HG11	1:A:854:LYS:HE2	1.92	0.51
2:B:543:VAL:HG11	2:B:703:LEU:HG	1.92	0.51
1:A:907:ILE:HD11	2:B:342:VAL:HB	1.91	0.51
1:A:982:HIS:C	1:A:984:PRO:HD2	2.35	0.51
2:B:647:LYS:HD2	2:B:647:LYS:N	2.26	0.51
2:B:413:LEU:HD11	2:B:532:LYS:HD3	1.91	0.51
2:B:505:LEU:HB3	2:B:509:TRP:CD1	2.45	0.51
1:A:1024:ASP:CG	2:B:316:ARG:HH22	2.18	0.51
2:B:481:GLU:O	2:B:485:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:552:PRO:HD2	2:B:602:LYS:O	2.11	0.51
2:B:579:PHE:CD1	2:B:716:ILE:HG12	2.45	0.51
2:B:691:PRO:HB3	2:B:700:ARG:NE	2.25	0.51
2:B:143:ILE:HD12	2:B:146:ASN:OD1	2.10	0.51
2:B:363:LEU:HG	2:B:364:PRO:HD2	1.93	0.51
1:A:993:SER:HB3	1:A:996:GLU:CG	2.41	0.51
2:B:448:CYS:HA	2:B:451:ILE:HG12	1.93	0.51
2:B:543:VAL:HG21	2:B:703:LEU:HD23	1.91	0.51
2:B:688:ASN:H	2:B:689:PRO:CD	2.24	0.50
2:B:524:ASN:C	2:B:524:ASN:HD22	2.17	0.50
2:B:329:LYS:HB3	2:B:357:TRP:NE1	2.27	0.50
2:B:401:SER:HA	2:B:407:HIS:HD2	1.77	0.50
2:B:532:LYS:HE3	2:B:557:TYR:CE1	2.46	0.50
1:A:819:GLU:HA	1:A:822:ARG:HD2	1.93	0.50
1:A:980:LEU:HB3	1:A:983:PRO:HG2	1.92	0.50
1:A:982:HIS:N	1:A:983:PRO:CD	2.74	0.50
2:B:189:ILE:HD11	2:B:257:LEU:HD21	1.92	0.50
2:B:209:GLU:HA	2:B:214:LEU:HB2	1.93	0.50
2:B:408:ASP:O	2:B:412:LYS:HG3	2.11	0.50
2:B:185:LEU:HD23	2:B:208:PHE:HE2	1.76	0.50
1:A:800:LYS:HD3	1:A:822:ARG:NH2	2.26	0.50
2:B:297:ASN:HB2	2:B:298:PRO:HD3	1.93	0.50
2:B:164:VAL:HG11	2:B:610:SER:OG	2.11	0.50
2:B:167:ARG:HB2	2:B:687:THR:OG1	2.11	0.50
2:B:691:PRO:HB3	2:B:700:ARG:HE	1.77	0.50
1:A:805:HIS:CG	1:A:806:SER:N	2.77	0.49
2:B:215:TYR:H	2:B:222:SER:HB2	1.77	0.49
2:B:327:LYS:HB2	2:B:328:PRO:CD	2.35	0.49
1:A:972:LYS:O	1:A:974:PRO:HD3	2.13	0.49
2:B:169:LYS:NZ	2:B:682:LYS:HD2	2.28	0.49
2:B:189:ILE:HD11	2:B:257:LEU:CD2	2.43	0.49
1:A:800:LYS:NZ	1:A:857:LEU:HB3	2.28	0.48
2:B:173:MET:HA	2:B:629:GLU:O	2.12	0.48
2:B:307:ARG:HG2	2:B:307:ARG:HH11	1.78	0.48
2:B:315:TRP:CD1	2:B:369:PRO:HG2	2.48	0.48
2:B:688:ASN:HB2	2:B:689:PRO:HD3	1.96	0.48
1:A:1037:ARG:HA	1:A:1037:ARG:NE	2.28	0.48
2:B:613:HIS:O	2:B:617:ARG:HG3	2.13	0.48
1:A:980:LEU:HB3	1:A:983:PRO:CG	2.43	0.48
2:B:460:LYS:HG3	2:B:462:LYS:HE2	1.96	0.48
2:B:319:LEU:N	2:B:319:LEU:HD23	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:ASN:ND2	2:B:358:ASN:N	2.61	0.48
2:B:685:ILE:HD13	2:B:685:ILE:C	2.39	0.48
2:B:262:LEU:HD13	2:B:298:PRO:HB2	1.94	0.48
2:B:305:VAL:HB	2:B:309:TRP:CE2	2.48	0.48
2:B:159:LYS:HD3	2:B:609:PRO:HG3	1.96	0.48
2:B:185:LEU:HD23	2:B:208:PHE:CE2	2.49	0.48
2:B:506:TYR:HE1	2:B:522:LEU:HB3	1.78	0.48
2:B:176:VAL:HG22	2:B:216:PRO:HB3	1.95	0.48
2:B:316:ARG:CD	2:B:360:ASN:HB3	2.39	0.48
2:B:512:LEU:HD23	2:B:512:LEU:C	2.39	0.48
2:B:603:LEU:HB3	2:B:631:CYS:SG	2.54	0.48
1:A:914:LEU:HD13	1:A:916:PRO:HD3	1.95	0.47
2:B:440:THR:HG21	2:B:569:LEU:HG	1.97	0.47
1:A:876:LYS:O	1:A:880:GLU:HG2	2.15	0.47
1:A:918:LYS:HB2	1:A:922:GLU:CG	2.36	0.47
1:A:1028:PHE:HB3	1:A:1031:ASP:HB3	1.96	0.47
2:B:151:ILE:HG21	2:B:531:TYR:CD1	2.49	0.47
1:A:800:LYS:HB3	1:A:822:ARG:NE	2.30	0.46
1:A:983:PRO:CB	1:A:1052:CYS:HB3	2.45	0.46
2:B:560:SER:C	2:B:562:GLU:H	2.23	0.46
1:A:901:LYS:HD2	1:A:1011:ARG:NE	2.30	0.46
2:B:410:ILE:C	2:B:410:ILE:HD12	2.40	0.46
2:B:424:ILE:HD12	2:B:424:ILE:N	2.29	0.46
2:B:152:PRO:CG	2:B:431:ARG:HD2	2.39	0.46
2:B:508:LYS:O	2:B:511:PRO:HD2	2.16	0.46
2:B:325:ILE:HB	2:B:328:PRO:HD2	1.97	0.46
1:A:935:GLU:O	1:A:937:ILE:HG13	2.15	0.46
2:B:470:GLU:HA	2:B:473:LYS:HE2	1.97	0.46
1:A:968:LEU:HD12	1:A:1005:PHE:CG	2.51	0.46
2:B:184:LYS:HD3	2:B:396:THR:HG21	1.97	0.46
2:B:204:SER:HA	2:B:598:SER:OG	2.16	0.46
2:B:509:TRP:HB3	2:B:513:PHE:CE2	2.45	0.46
1:A:968:LEU:C	1:A:970:GLU:H	2.24	0.45
2:B:212:LEU:CD1	2:B:254:MET:HG3	2.47	0.45
2:B:299:LEU:HD11	2:B:375:MET:HG2	1.98	0.45
2:B:373:ARG:H	2:B:373:ARG:CD	2.18	0.45
2:B:460:LYS:NZ	2:B:460:LYS:HB3	2.31	0.45
1:A:867:PRO:O	1:A:868:LEU:C	2.58	0.45
2:B:142:LEU:HD21	2:B:517:LEU:HG	1.98	0.45
1:A:1051:GLN:O	1:A:1054:GLU:HB3	2.16	0.45
2:B:142:LEU:HD23	2:B:143:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:ARG:HD3	2:B:373:ARG:N	2.27	0.45
1:A:858:LEU:O	1:A:862:VAL:HG23	2.16	0.45
2:B:414:THR:HG23	2:B:415:HIS:CD2	2.52	0.45
2:B:422:PHE:HE1	2:B:531:TYR:HE1	1.63	0.45
2:B:168:LEU:HD12	2:B:168:LEU:N	2.32	0.45
1:A:850:GLU:OE2	1:A:854:LYS:HE3	2.17	0.45
2:B:141:ALA:O	2:B:454:ARG:HD3	2.17	0.45
2:B:206:GLN:NE2	2:B:602:LYS:HG2	2.32	0.45
2:B:431:ARG:HG3	2:B:435:GLU:HG3	1.99	0.45
2:B:383:LEU:N	2:B:383:LEU:HD22	2.32	0.44
1:A:978:LEU:HD23	1:A:978:LEU:C	2.42	0.44
1:A:1012:ASP:O	1:A:1014:VAL:HG23	2.17	0.44
2:B:146:ASN:HD22	2:B:146:ASN:N	2.14	0.44
1:A:799:PRO:HB2	1:A:800:LYS:H	1.59	0.44
1:A:824:TRP:CE2	1:A:867:PRO:HD3	2.51	0.44
2:B:685:ILE:HG12	2:B:687:THR:HG22	2.00	0.44
2:B:321:SER:O	2:B:322:ASP:HB2	2.17	0.44
2:B:420:PRO:HG3	2:B:530:LEU:HD11	1.99	0.44
1:A:961:GLN:NE2	1:A:1009:LEU:HG	2.32	0.44
1:A:982:HIS:N	1:A:983:PRO:HD2	2.33	0.44
2:B:551:MET:HE3	2:B:553:ARG:HG3	2.00	0.44
1:A:818:TYR:C	1:A:820:LYS:H	2.25	0.44
1:A:869:THR:HG22	1:A:870:GLU:N	2.32	0.44
1:A:800:LYS:N	1:A:801:PRO:HD3	2.32	0.44
2:B:236:LEU:O	2:B:236:LEU:HD22	2.18	0.44
2:B:212:LEU:HD12	2:B:212:LEU:N	2.33	0.43
2:B:319:LEU:HD23	2:B:319:LEU:H	1.82	0.43
2:B:690:LEU:C	2:B:690:LEU:HD13	2.43	0.43
1:A:919:THR:HG23	1:A:921:GLU:H	1.84	0.43
1:A:964:LEU:CD2	1:A:1005:PHE:HB2	2.48	0.43
2:B:606:HIS:CD2	2:B:608:THR:HG23	2.54	0.43
2:B:399:CYS:O	2:B:403:SER:HB3	2.19	0.43
2:B:506:TYR:CE1	2:B:522:LEU:HB3	2.54	0.43
2:B:554:LEU:H	2:B:598:SER:CB	2.26	0.43
2:B:151:ILE:HG13	2:B:531:TYR:CG	2.54	0.43
1:A:1025:CYS:HA	1:A:1026:PRO:HD3	1.79	0.43
2:B:186:MET:CE	2:B:552:PRO:HB3	2.48	0.43
1:A:920:LEU:C	1:A:920:LEU:HD23	2.43	0.43
2:B:716:ILE:HD12	2:B:720:PHE:CE2	2.53	0.43
2:B:174:LYS:HA	2:B:175:PRO:HD3	1.90	0.43
2:B:314:GLU:HG3	2:B:390:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:PRO:O	1:A:1029:GLU:HB2	2.19	0.43
2:B:178:TYR:CZ	2:B:214:LEU:HB3	2.53	0.43
2:B:554:LEU:HB2	2:B:598:SER:HB2	1.99	0.43
1:A:999:PHE:CZ	1:A:1003:MET:HE3	2.54	0.42
2:B:153:LEU:HD23	2:B:153:LEU:N	2.27	0.42
2:B:224:ALA:HB3	2:B:235:LEU:HD22	2.00	0.42
2:B:330:THR:O	2:B:331:ALA:HB2	2.19	0.42
1:A:875:MET:HB3	1:A:879:TRP:CD1	2.54	0.42
2:B:167:ARG:C	2:B:168:LEU:HD12	2.44	0.42
2:B:265:THR:HB	2:B:399:CYS:HA	2.01	0.42
2:B:444:PHE:CE1	2:B:522:LEU:HD12	2.55	0.42
2:B:688:ASN:H	2:B:689:PRO:HD2	1.84	0.42
2:B:164:VAL:HG21	2:B:610:SER:OG	2.19	0.42
2:B:383:LEU:HD22	2:B:383:LEU:H	1.84	0.42
1:A:912:ARG:HD3	1:A:912:ARG:C	2.45	0.42
2:B:651:PRO:HG2	2:B:691:PRO:O	2.20	0.42
2:B:579:PHE:CE2	2:B:589:LEU:HD11	2.55	0.42
2:B:736:GLN:HA	2:B:739:ARG:HG2	2.01	0.42
1:A:1019:ARG:HD2	1:A:1019:ARG:C	2.45	0.41
1:A:902:TYR:CD1	1:A:909:ALA:HB1	2.55	0.41
2:B:188:PHE:HE2	2:B:196:PHE:HZ	1.68	0.41
2:B:292:LYS:C	2:B:294:VAL:H	2.28	0.41
2:B:611:LEU:HD13	2:B:611:LEU:C	2.46	0.41
1:A:807:HIS:CD2	1:A:938:GLU:HB2	2.55	0.41
1:A:866:GLN:CG	1:A:867:PRO:HD2	2.51	0.41
1:A:978:LEU:HB3	1:A:998:ARG:CD	2.50	0.41
2:B:318:GLN:C	2:B:320:PRO:HD3	2.46	0.41
2:B:432:TYR:CD2	2:B:569:LEU:HB2	2.55	0.41
2:B:159:LYS:HB3	2:B:159:LYS:HZ3	1.83	0.41
2:B:505:LEU:HB3	2:B:509:TRP:NE1	2.35	0.41
2:B:203:LEU:HD21	2:B:253:LYS:HB3	2.03	0.41
2:B:522:LEU:HD23	2:B:522:LEU:HA	1.91	0.41
1:A:835:MET:HA	1:A:838:VAL:HG12	2.02	0.41
2:B:354:ILE:N	2:B:354:ILE:HD12	2.36	0.41
2:B:611:LEU:HD23	2:B:626:TYR:CZ	2.56	0.41
1:A:1033:TYR:O	1:A:1037:ARG:HD2	2.21	0.41
2:B:472:LYS:O	2:B:476:LEU:HG	2.21	0.41
1:A:847:ASP:HB3	1:A:848:GLN:H	1.70	0.41
1:A:858:LEU:C	1:A:858:LEU:HD23	2.45	0.41
1:A:875:MET:O	1:A:876:LYS:C	2.64	0.41
2:B:150:VAL:CG1	2:B:431:ARG:H	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:LYS:HD2	2:B:355:TYR:CD2	2.56	0.41
1:A:916:PRO:HB2	1:A:917:GLY:H	1.56	0.41
1:A:1000:ILE:O	1:A:1004:LEU:HG	2.21	0.41
1:A:835:MET:HG3	1:A:854:LYS:NZ	2.35	0.40
2:B:482:ILE:HD12	2:B:512:LEU:HD12	2.02	0.40
2:B:731:LYS:N	2:B:731:LYS:HD2	2.36	0.40
1:A:884:PHE:C	1:A:886:ASN:H	2.29	0.40
1:A:964:LEU:HD23	1:A:964:LEU:C	2.46	0.40
1:A:983:PRO:N	1:A:984:PRO:CD	2.84	0.40
2:B:303:ARG:HG2	2:B:370:LEU:HD13	2.02	0.40
2:B:531:TYR:O	2:B:532:LYS:C	2.64	0.40
1:A:974:PRO:C	1:A:976:PHE:H	2.30	0.40
1:A:1037:ARG:HH12	2:B:410:ILE:HD11	1.87	0.40
2:B:279:GLY:O	2:B:281:LEU:HG	2.21	0.40
2:B:516:GLU:O	2:B:518:PRO:HD3	2.22	0.40
2:B:361:GLU:HA	2:B:361:GLU:OE1	2.21	0.40
2:B:705:ILE:HD12	2:B:705:ILE:C	2.46	0.40
2:B:506:TYR:O	2:B:510:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	275/374 (74%)	214 (78%)	52 (19%)	9 (3%)	3	18
2	B	588/624 (94%)	481 (82%)	92 (16%)	15 (3%)	4	21
All	All	863/998 (86%)	695 (80%)	144 (17%)	24 (3%)	4	20

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	799	PRO
1	A	916	PRO
1	A	904	ARG
1	A	793	PRO
2	B	162	TYR
2	B	232	ASP
2	B	331	ALA
2	B	339	THR
2	B	514	GLU
2	B	533	LEU
2	B	622	SER
2	B	690	LEU
2	B	692	LYS
1	A	868	LEU
1	A	914	LEU
2	B	376	ASP
1	A	830	GLY
1	A	986	SER
2	B	278	LYS
2	B	349	ILE
2	B	502	LEU
2	B	688	ASN
1	A	811	PRO
2	B	493	ALA

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	254/343 (74%)	249 (98%)	5 (2%)	48	66
2	B	543/571 (95%)	517 (95%)	26 (5%)	23	50
All	All	797/914 (87%)	766 (96%)	31 (4%)	28	54

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

Mol	Chain	Res	Type
1	A	914	LEU
1	A	937	ILE
1	A	987	ASN
1	A	1006	LYS
1	A	1037	ARG
2	B	153	LEU
2	B	159	LYS
2	B	165	ILE
2	B	167	ARG
2	B	228	LYS
2	B	236	LEU
2	B	237	LEU
2	B	255	ASN
2	B	265	THR
2	B	276	LYS
2	B	277	LYS
2	B	319	LEU
2	B	330	THR
2	B	353	ASN
2	B	358	ASN
2	B	370	LEU
2	B	373	ARG
2	B	381	LEU
2	B	413	LEU
2	B	447	LEU
2	B	520	GLN
2	B	557	TYR
2	B	644	LEU
2	B	685	ILE
2	B	716	ILE
2	B	727	PHE

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	805	HIS
1	A	807	HIS
1	A	808	GLN
1	A	863	ASN
1	A	905	ASN
1	A	961	GLN
1	A	982	HIS
1	A	987	ASN

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Mol	Chain	Res	Type
2	B	146	ASN
2	B	172	ASN
2	B	201	GLN
2	B	220	ASN
2	B	255	ASN
2	B	318	GLN
2	B	335	GLN
2	B	353	ASN
2	B	358	ASN
2	B	407	HIS
2	B	415	HIS
2	B	520	GLN
2	B	524	ASN
2	B	536	GLN
2	B	582	ASN
2	B	592	ASN
2	B	595	GLN
2	B	652	GLN
2	B	659	ASN
2	B	681	ASN
2	B	688	ASN
2	B	726	GLN
2	B	736	GLN
2	B	743	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	277/374 (74%)	0.54	18 (6%) 25 17	91, 154, 262, 349	0
2	B	592/624 (94%)	0.46	33 (5%) 30 20	79, 132, 259, 319	0
All	All	869/998 (87%)	0.49	51 (5%) 28 19	79, 138, 261, 349	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1041	GLU	4.6
2	B	268	GLU	4.6
2	B	619	ARG	4.4
1	A	915	ALA	4.3
1	A	856	GLU	4.3
2	B	321	SER	3.9
2	B	326	SER	3.8
2	B	319	LEU	3.7
1	A	916	PRO	3.7
1	A	932	SER	3.5
1	A	813	GLN	3.0
2	B	160	ASN	3.0
2	B	138	VAL	3.0
1	A	917	GLY	2.9
2	B	434	ILE	2.9
2	B	501	LEU	2.9
2	B	685	ILE	2.8
2	B	735	ARG	2.7
1	A	847	ASP	2.7
2	B	656	LYS	2.7
2	B	274	SER	2.7
2	B	287	LEU	2.6
1	A	833	PRO	2.5
1	A	835	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	153	LEU	2.5
1	A	853	GLU	2.5
1	A	884	PHE	2.4
2	B	582	ASN	2.4
2	B	729	ASP	2.4
2	B	521	PRO	2.4
2	B	152	PRO	2.4
2	B	339	THR	2.3
2	B	483	LEU	2.3
2	B	139	GLU	2.2
1	A	914	LEU	2.2
1	A	1014	VAL	2.2
1	A	1061	ILE	2.2
2	B	503	PHE	2.2
2	B	281	LEU	2.2
1	A	852	LYS	2.2
1	A	937	ILE	2.1
2	B	288	LYS	2.1
2	B	599	ALA	2.1
1	A	860	LEU	2.1
2	B	502	LEU	2.1
2	B	690	LEU	2.1
2	B	327	LYS	2.1
2	B	746	ASN	2.1
2	B	687	THR	2.1
2	B	620	ASN	2.0
2	B	141	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.