



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:47 am GMT

PDB ID : 2Y9Y  
Title : Chromatin Remodeling Factor ISW1a(del\_ATPase)  
Authors : Yamada, K.; Frouws, T.D.; Angst, B.; Fitzgerald, D.J.; Deluca, C.; Schimmele, 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

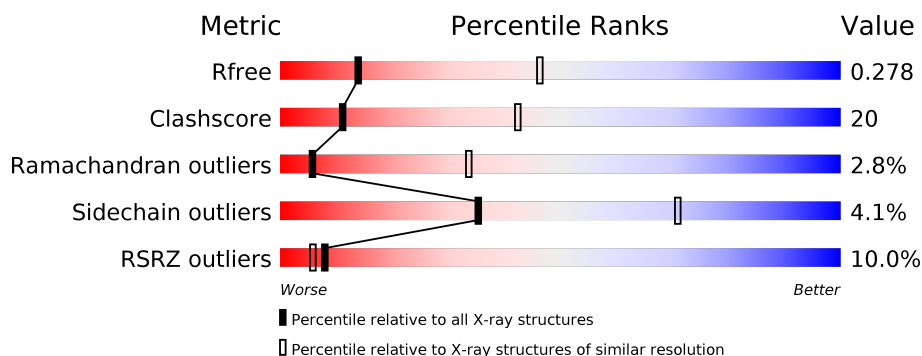
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
2	B	624	

## 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, $\alpha$ , $\beta$ , $\gamma$	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) 100.0 (29.87-3.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.93 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.283 , 0.296 0.275 , 0.278	Depositor DCC
$R_{free}$ test set	1380 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	120.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 97.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.21	0/2368	0.35	0/3186
2	B	0.21	0/4974	0.35	0/6723
All	All	0.21	0/7342	0.35	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	87	0
2	B	4853	0	4857	204	0
All	All	7170	0	7157	287	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 20.

All (287) 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:HD23	2:B:237:LEU:H	1.46	0.79
2:B:164:VAL:HG22	2:B:609:PRO:HB2	1.61	0.79
2:B:153:LEU:HD23	2:B:153:LEU:H	1.50	0.77
2:B:381:LEU:H	2:B:381:LEU:HD12	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:186:MET:HE1	2:B:205:PHE:HD2	1.63	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:N	2:B:353:ASN:HD22	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:HB3	2:B:159:LYS:NZ	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:O	1:A:807:HIS:CG	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:ND2	2:B:358:ASN:H	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:510:VAL:HB	2:B:511:PRO:HD3	1.87	0.56
2:B:151:ILE:HD11	2:B:525:PRO:HB3	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:476:LEU:HA	2:B:479:LYS:HD2	1.88	0.55
1:A:983:PRO:CA	1:A:1052:CYS:HB3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	2:B:245:LYS:O	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: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
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: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:140:PRO:HB3	2:B:457:ILE:HG12	1.91	0.52
2:B:149:SER:HB2	2:B:519:ASP:CB	2.40	0.52
2:B:167:ARG:H	2:B:167:ARG:CD	2.20	0.52
2:B:150:VAL:HG22	2:B:521:PRO:HA	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
2:B:647:LYS:HD2	2:B:647:LYS:N	2.26	0.51
2:B:505:LEU:HB3	2:B:509:TRP:CD1	2.45	0.51
2:B:413:LEU:HD11	2:B:532:LYS:HD3	1.91	0.51
2:B:481:GLU:O	2:B:485:GLU:HG2	2.11	0.51
2:B:552:PRO:HD2	2:B:602:LYS:O	2.11	0.51
2:B:691:PRO:HB3	2:B:700:ARG:NE	2.25	0.51
2:B:579:PHE:CD1	2:B:716:ILE:HG12	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:209:GLU:HA	2:B:214:LEU:HB2	1.93	0.50
2:B:189:ILE:HD11	2:B:257:LEU:HD21	1.92	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
2:B:186:MET:HE1	2:B:205:PHE:CD2	2.45	0.50
2:B:321:SER:C	2:B:323:GLN:H	2.15	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:167:ARG:HB2	2:B:687:THR:OG1	2.11	0.50
2:B:164:VAL:HG11	2:B:610:SER:OG	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:189:ILE:HD11	2:B:257:LEU:CD2	2.43	0.49
2:B:169:LYS:NZ	2:B:682:LYS:HD2	2.28	0.49
1:A:800:LYS:NZ	1:A:857:LEU:HB3	2.28	0.48
2:B:307:ARG:HH11	2:B:307:ARG:HG2	1.78	0.48
2:B:173:MET:HA	2:B:629:GLU:O	2.12	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:NE	1:A:1037:ARG:HA	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
2:B:358:ASN:ND2	2:B:358:ASN:N	2.61	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:537:GLU:H	2:B:537:GLU:CD	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LYS:HD3	2:B:609:PRO:HG3	1.96	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: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
2:B:537:GLU:C	2:B:539:PHE:H	2.18	0.47
1:A:876:LYS:O	1:A:880:GLU:HG2	2.15	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:918:LYS:HB2	1:A:922:GLU:CG	2.36	0.47
1:A:982:HIS:C	1:A:984:PRO:HD2	2.35	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
1:A:901:LYS:HD2	1:A:1011:ARG:NE	2.30	0.46
2:B:524:ASN:HD22	2:B:524:ASN:C	2.17	0.46
2:B:424:ILE:HD12	2:B:424:ILE:N	2.29	0.46
1:A:1024:ASP:CG	2:B:316:ARG:HH22	2.18	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:204:SER:HA	2:B:598:SER:OG	2.16	0.46
2:B:184:LYS:HD3	2:B:396:THR:HG21	1.97	0.46
2:B:509:TRP:HB3	2:B:513:PHE:CE2	2.45	0.46
2:B:212:LEU:CD1	2:B:254:MET:HG3	2.47	0.45
2:B:373:ARG:H	2:B:373:ARG:CD	2.18	0.45
2:B:299:LEU:HD11	2:B:375:MET:HG2	1.98	0.45
2:B:460:LYS:HB3	2:B:460:LYS:NZ	2.31	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
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:206:GLN:NE2	2:B:602:LYS:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ARG:HG3	2:B:435:GLU:HG3	1.99	0.45
2:B:141:ALA:O	2:B:454:ARG:HD3	2.17	0.45
2:B:383:LEU:HD22	2:B:383:LEU:N	2.32	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
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:H	2:B:319:LEU:HD23	1.82	0.43
1:A:964:LEU:CD2	1:A:1005:PHE:HB2	2.48	0.43
1:A:919:THR:HG23	1:A:921:GLU:H	1.84	0.43
2:B:606:HIS:CD2	2:B:608:THR:HG23	2.54	0.43
2:B:685:ILE:C	2:B:685:ILE:HD13	2.39	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
2:B:512:LEU:HD23	2:B:512:LEU:C	2.39	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
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
2:B:153:LEU:N	2:B:153:LEU:HD23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:VAL:HG21	2:B:610:SER:OG	2.19	0.42
2:B:383:LEU:H	2:B:383:LEU:HD22	1.84	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
2:B:560:SER:C	2:B:562:GLU:H	2.23	0.42
2:B:173:MET:HE2	2:B:630:LEU:CD2	2.50	0.41
2:B:410:ILE:C	2:B:410:ILE:HD12	2.40	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
1:A:866:GLN:CG	1:A:867:PRO:HD2	2.51	0.41
1:A:807:HIS:CD2	1:A:938:GLU:HB2	2.55	0.41
1:A:978:LEU:HB3	1:A:998:ARG:CD	2.50	0.41
2:B:432:TYR:CD2	2:B:569:LEU:HB2	2.55	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:968:LEU:C	1:A:970:GLU:H	2.24	0.41
2:B:329:LYS:HD2	2:B:355:TYR:CD2	2.56	0.41
2:B:150:VAL:CG1	2:B:431:ARG:H	2.30	0.41
1:A:847:ASP:HB3	1:A:848:GLN:H	1.70	0.41
1:A:1000:ILE:O	1:A:1004:LEU:HG	2.21	0.41
1:A:867:PRO:O	1:A:868:LEU:C	2.58	0.41
1:A:916:PRO:HB2	1:A:917:GLY:H	1.56	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:HD2	2:B:731:LYS:N	2.36	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
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:OE1	2:B:361:GLU:HA	2.21	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%)	4	29
2	B	588/624 (94%)	481 (82%)	92 (16%)	15 (3%)	6	35
All	All	863/998 (86%)	695 (80%)	144 (17%)	24 (3%)	6	34

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%)	250 (98%)	4 (2%)	68	86
2	B	543/571 (95%)	514 (95%)	29 (5%)	26	64
All	All	797/914 (87%)	764 (96%)	33 (4%)	35	71

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	822	ARG
1	A	914	LEU
1	A	987	ASN
1	A	1037	ARG
2	B	159	LYS
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	273	LYS
2	B	276	LYS
2	B	284	TRP
2	B	319	LEU
2	B	330	THR
2	B	353	ASN
2	B	358	ASN
2	B	373	ARG
2	B	381	LEU
2	B	413	LEU
2	B	447	LEU
2	B	458	ARG
2	B	520	GLN
2	B	524	ASN
2	B	557	TYR
2	B	605	TYR

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Mol	Chain	Res	Type
2	B	619	ARG
2	B	644	LEU
2	B	685	ILE
2	B	716	ILE
2	B	727	PHE
2	B	739	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	908	GLN
1	A	961	GLN
1	A	973	ASN
1	A	987	ASN
2	B	160	ASN
2	B	172	ASN
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	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 [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 carbohydrates 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/374 (74%)	0.46	27 (9%) 8 6	91, 154, 262, 349	0
2	B	592/624 (94%)	0.51	60 (10%) 8 5	79, 132, 259, 319	0
All	All	869/998 (87%)	0.50	87 (10%) 8 6	79, 138, 261, 349	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	274	SER	11.3
2	B	139	GLU	9.8
2	B	469	LYS	8.9
2	B	275	ALA	8.3
2	B	470	GLU	8.1
2	B	494	VAL	7.9
1	A	798	MET	7.3
2	B	680	ASP	5.9
2	B	468	LEU	5.8
2	B	467	GLN	5.6
2	B	280	PRO	5.3
1	A	791	SER	5.2
1	A	799	PRO	5.1
2	B	681	ASN	5.1
2	B	659	ASN	5.0
2	B	495	LYS	4.8
2	B	457	ILE	4.8
1	A	847	ASP	4.6
2	B	493	ALA	4.6
2	B	503	PHE	4.5
1	A	836	ASP	4.4
1	A	794	SER	4.3
1	A	942	LYS	4.3
1	A	866	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	661	LYS	4.2
2	B	658	GLY	4.2
2	B	471	GLY	4.2
2	B	679	THR	4.1
2	B	491	LYS	4.1
1	A	918	LYS	4.0
2	B	472	LYS	4.0
2	B	273	LYS	3.9
2	B	660	GLU	3.9
2	B	653	ASP	3.8
1	A	1067	THR	3.7
2	B	320	PRO	3.7
2	B	655	LYS	3.5
2	B	746	ASN	3.5
2	B	656	LYS	3.4
2	B	496	SER	3.4
2	B	498	LYS	3.4
2	B	499	ASP	3.3
2	B	459	SER	3.3
2	B	276	LYS	3.3
2	B	464	PHE	3.2
1	A	795	HIS	3.2
1	A	802	HIS	3.2
2	B	466	LYS	3.2
1	A	848	GLN	3.1
1	A	1064	ASP	3.1
2	B	492	ASN	3.1
2	B	162	TYR	3.1
2	B	650	LYS	3.0
1	A	804	PHE	3.0
2	B	417	LYS	2.9
2	B	278	LYS	2.9
1	A	917	GLY	2.9
1	A	792	THR	2.9
2	B	683	PRO	2.9
2	B	138	VAL	2.9
1	A	1055	LYS	2.8
1	A	835	MET	2.8
2	B	745	VAL	2.8
2	B	230	PRO	2.8
2	B	742	ARG	2.8
2	B	279	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	797	ARG	2.8
1	A	793	PRO	2.7
1	A	1066	ALA	2.6
2	B	620	ASN	2.6
2	B	654	GLU	2.6
2	B	686	ASN	2.6
2	B	489	GLU	2.5
2	B	484	LYS	2.5
2	B	487	LYS	2.4
2	B	153	LEU	2.4
2	B	321	SER	2.4
1	A	845	ILE	2.4
1	A	1065	ASP	2.4
1	A	915	ALA	2.3
2	B	473	LYS	2.2
2	B	657	GLU	2.2
2	B	455	TYR	2.1
1	A	813	GLN	2.1
2	B	233	THR	2.1
1	A	1063	LEU	2.1
2	B	501	LEU	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 carbohydrates 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.