Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID	:	1XEW
Title	:	Structural biochemistry of ATP-driven dimerization and DNA stimulated activation of SMC ATPases.
Authors	:	Lammens, A.; Schele, A.; Hopfner, K.-P.
Deposited on	:	2004-09-13
Resolution	:	2.00 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.
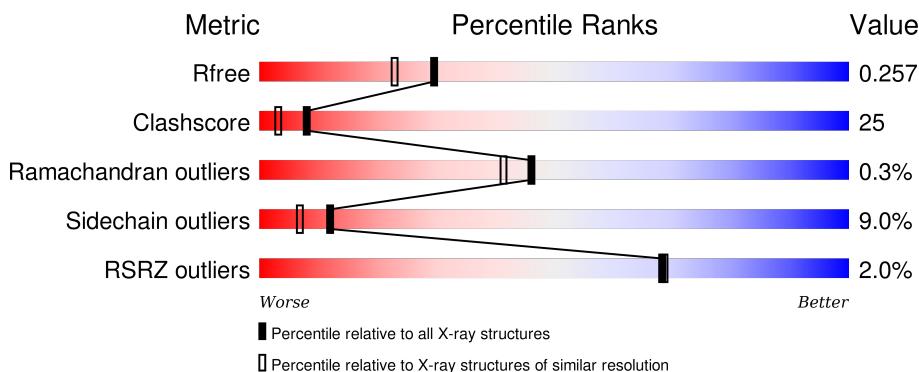
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 >=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 <=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	X	182	56% 19% 6% 19%
2	Y	172	63% 23% 8% 7%
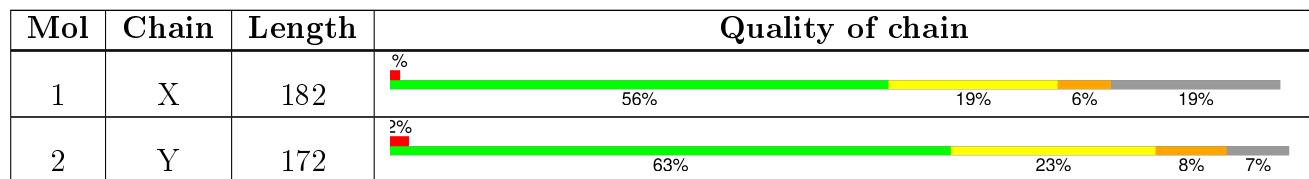
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2710 atoms, of which 4 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 SMC protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	X	147	Total	C	H	N	O	S	21	0	0
			1158	741	4	197	213	3			

- Molecule 2 is a protein called SMC protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	160	Total	C	N	O	S	3	0	0
			1242	799	207	230	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	173	Total	O	0	0
			173	173		
3	Y	137	Total	O	0	0
			137	137		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: SMC protein
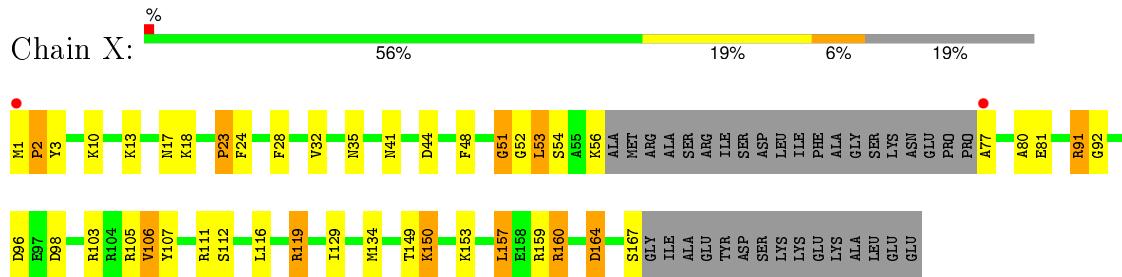
- Molecule 2: SMC protein
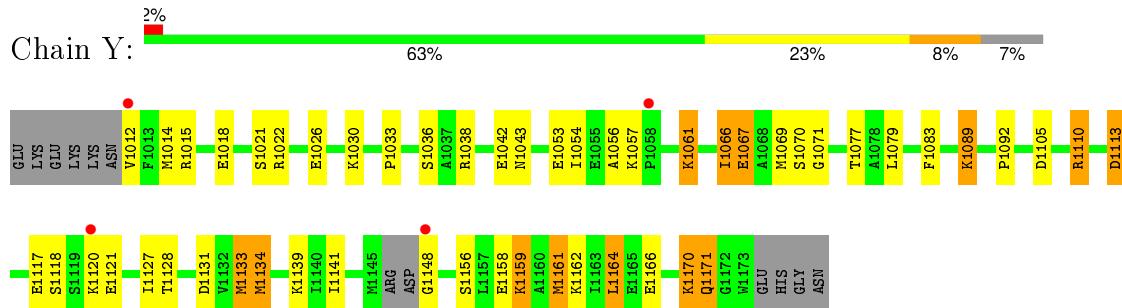
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	102.28Å 56.74Å 78.87Å 90.00° 123.05° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 33.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 88.0 (33.94-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	6.49 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.261 0.233 , 0.257	Depositor DCC
R_{free} test set	1101 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 86.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 22600 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2710	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	X	1.25	2/1174 (0.2%)	1.14	7/1579 (0.4%)
2	Y	1.19	0/1261	1.05	0/1689
All	All	1.22	2/2435 (0.1%)	1.10	7/3268 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	54	SER	CB-OG	8.13	1.52	1.42
1	X	112	SER	CB-OG	5.42	1.49	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	160	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	X	91	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	X	164	ASP	CB-CG-OD2	6.44	124.10	118.30
1	X	51	GLY	N-CA-C	6.13	128.44	113.10
1	X	119	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	X	91	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	X	160	ARG	NE-CZ-NH2	5.38	122.99	120.30

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	X	1154	4	1181	61	0
2	Y	1242	0	1283	69	0
3	X	173	0	0	28	1
3	Y	137	0	0	25	0
All	All	2706	4	2464	119	1

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 25.

All (119) 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:X:53:LEU:H	1:X:53:LEU:CD2	1.50	1.23
1:X:53:LEU:H	1:X:53:LEU:HD22	1.21	1.06
2:Y:1139:LYS:HZ2	2:Y:1141:ILE:HD11	1.19	1.06
1:X:10:LYS:HG3	3:X:343:HOH:O	1.57	1.04
1:X:157:LEU:HD12	3:X:355:HOH:O	1.58	1.01
2:Y:1026:GLU:HG3	3:Y:307:HOH:O	1.60	1.01
2:Y:1139:LYS:NZ	2:Y:1141:ILE:HD11	1.75	1.00
2:Y:1089:LYS:HE2	3:Y:287:HOH:O	1.65	0.96
1:X:35:ASN:H	2:Y:1171:GLN:HE22	1.11	0.92
1:X:53:LEU:N	1:X:53:LEU:CD2	2.32	0.90
3:X:330:HOH:O	2:Y:1067:GLU:HG3	1.70	0.89
1:X:105:ARG:HB3	3:X:346:HOH:O	1.72	0.89
1:X:53:LEU:H	1:X:53:LEU:HD23	1.38	0.88
1:X:1:MET:HB3	2:Y:1092:PRO:HB3	1.55	0.87
1:X:53:LEU:HB2	3:X:348:HOH:O	1.74	0.87
2:Y:1139:LYS:HZ2	2:Y:1141:ILE:CD1	1.91	0.84
1:X:134:MET:HE3	3:Y:287:HOH:O	1.76	0.84
2:Y:1134:MET:SD	2:Y:1164:LEU:HD13	2.20	0.81
2:Y:1113:ASP:O	2:Y:1117:GLU:HG2	1.81	0.80
2:Y:1033:PRO:HG3	2:Y:1110:ARG:HH11	1.45	0.80
1:X:81:GLU:OE2	1:X:103:ARG:HD3	1.82	0.77
2:Y:1121:GLU:HG3	3:Y:116:HOH:O	1.83	0.76
2:Y:1156:SER:OG	2:Y:1159:LYS:HG2	1.85	0.76
2:Y:1054:ILE:HB	2:Y:1066:ILE:HG12	1.68	0.74
2:Y:1117:GLU:HB3	3:Y:100:HOH:O	1.85	0.74
2:Y:1134:MET:CE	2:Y:1164:LEU:HD13	2.17	0.74
1:X:53:LEU:HD22	1:X:53:LEU:N	1.99	0.74
2:Y:1033:PRO:CG	2:Y:1110:ARG:HH11	2.00	0.73
2:Y:1148:GLY:HA2	3:Y:308:HOH:O	1.88	0.73
1:X:23:PRO:HG2	2:Y:1139:LYS:HZ3	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1158:GLU:H	2:Y:1158:GLU:CD	1.91	0.72
2:Y:1113:ASP:HB2	3:Y:309:HOH:O	1.89	0.71
2:Y:1162:LYS:O	2:Y:1166:GLU:HG3	1.91	0.71
2:Y:1110:ARG:HG3	3:Y:276:HOH:O	1.91	0.71
2:Y:1158:GLU:HG2	3:Y:266:HOH:O	1.91	0.70
2:Y:1061:LYS:HE2	3:Y:163:HOH:O	1.90	0.70
1:X:23:PRO:HG2	2:Y:1139:LYS:NZ	2.06	0.70
1:X:91:ARG:NH1	1:X:98:ASP:OD1	2.25	0.70
2:Y:1113:ASP:CB	3:Y:309:HOH:O	2.40	0.69
1:X:80:ALA:HB3	1:X:106:VAL:HG23	1.73	0.69
1:X:106:VAL:CG1	3:X:336:HOH:O	2.41	0.68
1:X:18:LYS:HE2	3:X:345:HOH:O	1.93	0.68
1:X:18:LYS:CE	3:X:345:HOH:O	2.41	0.68
2:Y:1089:LYS:HG2	3:Y:319:HOH:O	1.94	0.67
3:X:330:HOH:O	2:Y:1067:GLU:CG	2.38	0.67
2:Y:1089:LYS:HG3	3:Y:63:HOH:O	1.95	0.65
2:Y:1026:GLU:CG	3:Y:307:HOH:O	2.31	0.65
2:Y:1079:LEU:HD21	2:Y:1083:PHE:CE1	2.32	0.64
1:X:17:ASN:C	3:X:343:HOH:O	2.35	0.64
1:X:119:ARG:NH2	3:X:337:HOH:O	2.30	0.63
2:Y:1134:MET:SD	2:Y:1164:LEU:CD1	2.85	0.63
1:X:80:ALA:HB3	1:X:106:VAL:CG2	2.28	0.63
1:X:51:GLY:HA2	3:X:353:HOH:O	1.99	0.62
1:X:18:LYS:HD3	3:X:326:HOH:O	2.00	0.61
1:X:53:LEU:N	1:X:53:LEU:HD23	2.09	0.61
2:Y:1089:LYS:NZ	3:Y:319:HOH:O	2.34	0.60
2:Y:1012:VAL:N	3:Y:304:HOH:O	2.33	0.60
1:X:23:PRO:O	2:Y:1139:LYS:NZ	2.28	0.60
1:X:105:ARG:CB	3:X:346:HOH:O	2.38	0.60
1:X:35:ASN:H	2:Y:1171:GLN:NE2	1.92	0.59
1:X:2:PRO:HD3	1:X:92:GLY:HA3	1.84	0.58
2:Y:1079:LEU:CD2	2:Y:1083:PHE:CE1	2.86	0.58
1:X:13:LYS:NZ	1:X:44:ASP:OD2	2.36	0.58
1:X:3:TYR:HD2	3:X:286:HOH:O	1.86	0.57
2:Y:1079:LEU:HD21	2:Y:1083:PHE:CZ	2.40	0.56
1:X:150:LYS:HD2	3:X:242:HOH:O	2.05	0.56
1:X:18:LYS:NZ	3:X:334:HOH:O	2.39	0.56
1:X:52:GLY:C	3:X:193:HOH:O	2.45	0.55
2:Y:1042:GLU:OE2	2:Y:1053:GLU:OE1	2.24	0.55
1:X:1:MET:HB3	2:Y:1092:PRO:CB	2.32	0.55
2:Y:1131:ASP:OD1	2:Y:1161:MET:CG	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1089:LYS:CG	3:Y:319:HOH:O	2.52	0.54
2:Y:1015:ARG:HD3	3:Y:120:HOH:O	2.06	0.54
2:Y:1131:ASP:OD1	2:Y:1161:MET:HG3	2.07	0.54
1:X:91:ARG:NH2	1:X:96:ASP:OD2	2.41	0.53
1:X:77:ALA:HB3	3:X:240:HOH:O	2.08	0.53
1:X:106:VAL:HG12	3:X:336:HOH:O	2.06	0.53
2:Y:1030:LYS:O	2:Y:1110:ARG:HG2	2.08	0.53
2:Y:1033:PRO:HG3	2:Y:1110:ARG:NH1	2.22	0.51
1:X:149:THR:HG22	1:X:153:LYS:HD3	1.93	0.50
1:X:111:ARG:HD2	3:X:213:HOH:O	2.11	0.50
1:X:159:ARG:NH1	2:Y:1066:ILE:CD1	2.74	0.50
1:X:167:SER:C	3:X:339:HOH:O	2.51	0.49
1:X:48:PHE:CZ	1:X:106:VAL:HG22	2.48	0.48
1:X:48:PHE:HZ	1:X:106:VAL:HG22	1.78	0.48
1:X:56:LYS:HE3	3:X:311:HOH:O	2.14	0.47
2:Y:1089:LYS:CE	3:Y:287:HOH:O	2.40	0.47
2:Y:1148:GLY:CA	3:Y:308:HOH:O	2.57	0.47
1:X:24:PHE:HA	2:Y:1139:LYS:HE2	1.97	0.47
2:Y:1170:LYS:HA	2:Y:1170:LYS:HD2	1.68	0.47
1:X:56:LYS:NZ	3:X:325:HOH:O	2.31	0.46
1:X:53:LEU:HB3	3:X:191:HOH:O	2.14	0.46
1:X:18:LYS:CD	3:X:326:HOH:O	2.60	0.46
1:X:160:ARG:HD2	1:X:164:ASP:OD2	2.16	0.46
1:X:116:LEU:CD2	1:X:129:ILE:HD13	2.46	0.45
2:Y:1038:ARG:HD2	3:Y:289:HOH:O	2.16	0.45
2:Y:1110:ARG:CG	3:Y:276:HOH:O	2.57	0.45
2:Y:1036:SER:HA	3:Y:10:HOH:O	2.17	0.45
1:X:2:PRO:CD	1:X:92:GLY:HA3	2.45	0.44
2:Y:1014:MET:O	2:Y:1018:GLU:HG3	2.17	0.44
2:Y:1156:SER:HB2	2:Y:1158:GLU:OE2	2.17	0.44
1:X:149:THR:CG2	1:X:153:LYS:HD3	2.47	0.44
2:Y:1127:ILE:CD1	3:Y:90:HOH:O	2.66	0.44
1:X:28:PHE:HZ	2:Y:1133:MET:HE2	1.82	0.44
1:X:32:VAL:HG21	2:Y:1134:MET:SD	2.58	0.44
2:Y:1134:MET:HE1	2:Y:1164:LEU:HD13	1.98	0.43
2:Y:1054:ILE:HG21	2:Y:1077:THR:CG2	2.48	0.43
1:X:18:LYS:HB2	1:X:18:LYS:HE3	1.88	0.43
2:Y:1018:GLU:O	2:Y:1022:ARG:HG3	2.18	0.43
1:X:107:TYR:OH	3:X:198:HOH:O	2.22	0.42
2:Y:1056:ALA:HB3	2:Y:1069:MET:CE	2.49	0.42
1:X:116:LEU:HD22	1:X:129:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2:PRO:HA	3:X:286:HOH:O	2.19	0.41
2:Y:1158:GLU:CG	3:Y:266:HOH:O	2.58	0.41
2:Y:1070:SER:O	2:Y:1071:GLY:C	2.58	0.41
2:Y:1079:LEU:HD23	2:Y:1083:PHE:CE1	2.56	0.41
2:Y:1128:THR:HG21	2:Y:1133:MET:HB3	2.03	0.40
2:Y:1057:LYS:HE3	2:Y:1061:LYS:O	2.21	0.40
1:X:13:LYS:HD3	1:X:41:ASN:ND2	2.37	0.40

All (1) 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)
3:X:191:HOH:O	3:X:191:HOH:O[2_657]	1.76	0.44

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	X	143/182 (79%)	138 (96%)	4 (3%)	1 (1%)	26	19
2	Y	156/172 (91%)	154 (99%)	2 (1%)	0	100	100
All	All	299/354 (84%)	292 (98%)	6 (2%)	1 (0%)	46	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	2	PRO

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	X	123/151 (82%)	118 (96%)	5 (4%)	37	32
2	Y	133/144 (92%)	115 (86%)	18 (14%)	5	2
All	All	256/295 (87%)	233 (91%)	23 (9%)	12	7

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	23	PRO
1	X	53	LEU
1	X	106	VAL
1	X	150	LYS
1	X	157	LEU
2	Y	1021	SER
2	Y	1043	ASN
2	Y	1061	LYS
2	Y	1066	ILE
2	Y	1067	GLU
2	Y	1089	LYS
2	Y	1105	ASP
2	Y	1110	ARG
2	Y	1113	ASP
2	Y	1118	SER
2	Y	1120	LYS
2	Y	1133	MET
2	Y	1134	MET
2	Y	1159	LYS
2	Y	1161	MET
2	Y	1164	LEU
2	Y	1170	LYS
2	Y	1171	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	41	ASN
2	Y	1086	GLN
2	Y	1171	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, 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	X	147/182 (80%)	-0.07	2 (1%)	78	78	21, 32, 42, 50	4 (2%)
2	Y	160/172 (93%)	0.08	4 (2%)	61	61	23, 36, 48, 54	1 (0%)
All	All	307/354 (86%)	0.01	6 (1%)	68	69	21, 34, 46, 54	5 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1	MET	5.6
1	X	77	ALA	3.5
2	Y	1148	GLY	3.0
2	Y	1012	VAL	2.2
2	Y	1058	PRO	2.2
2	Y	1120	LYS	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.