Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2024 – 12:10 pm GMT

PDB ID	:	8OSB
Title	:	TWIST1-TCF4-ALX4 complex on specific DNA
Authors	:	Morgunova, E.; Kim, S.; Popov, A.; Wysocka, J.; Taipale, J.
Deposited on	:	2023-04-18
Resolution	:	2.90 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:

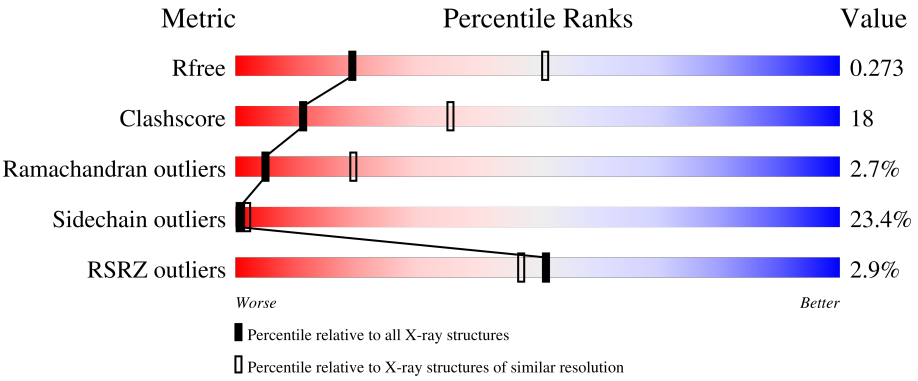
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	25	8% 64% 28%
2	W	25	20% 36% 44%
3	E	62	6% 60% 31% 10%
4	A	60	2% 55% 33% 12%
5	B	67	3% 54% 33% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2663 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 DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	25	518	248	97	148	25	0	0	0

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	W	25	507	245	85	152	25	0	0	0

- Molecule 3 is a protein called Homeobox protein aristaless-like 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	62	551	346	108	96	1	0	0	0

- Molecule 4 is a protein called Transcription factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	60	517	319	110	86	2	0	2	0

- Molecule 5 is a protein called Twist-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	66	543	342	97	103	1	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	X	12	12	12	0	0

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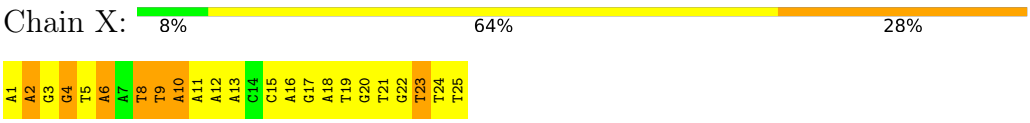
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	W	3	Total O 3 3	0	0
6	E	2	Total O 2 2	0	0
6	A	4	Total O 4 4	0	0
6	B	6	Total O 6 6	0	0

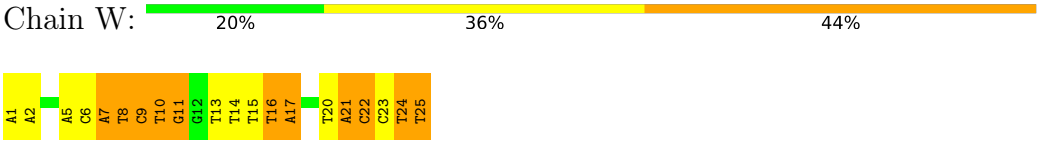
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

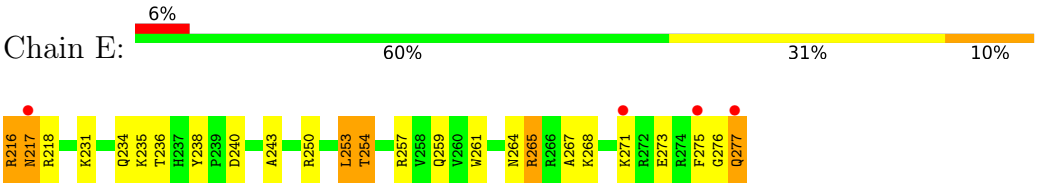
• Molecule 1: DNA (25-MER)



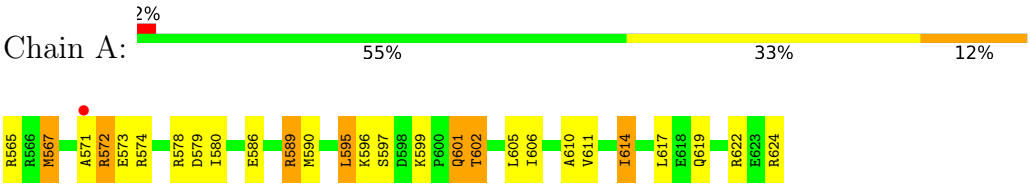
• Molecule 2: DNA (25-MER)



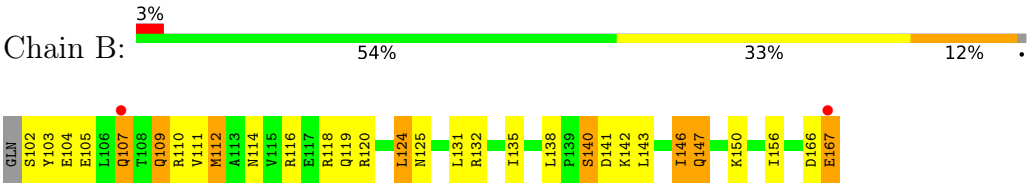
• Molecule 3: Homeobox protein aristaless-like 4



• Molecule 4: Transcription factor 4



• Molecule 5: Twist-related protein 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	60.59Å 60.59Å 237.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.00 – 2.90 47.99 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.00-2.90) 98.6 (47.99-2.83)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.220 , 0.270 0.225 , 0.273	Depositor DCC
R_{free} test set	635 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 70.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2663	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	X	1.07	0/582	1.81	20/897 (2.2%)
2	W	1.13	2/566 (0.4%)	1.86	20/870 (2.3%)
3	E	0.70	0/563	0.85	0/755
4	A	0.71	0/523	0.82	0/696
5	B	0.71	0/549	0.84	0/739
All	All	0.89	2/2783 (0.1%)	1.37	40/3957 (1.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	25	DT	P-O5'	6.46	1.66	1.59
2	W	22	DC	P-O5'	5.03	1.64	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	6	DC	P-O3'-C3'	-12.10	105.18	119.70
1	X	11	DA	P-O3'-C3'	-11.84	105.49	119.70
2	W	11	DG	P-O3'-C3'	-10.34	107.29	119.70
2	W	21	DA	P-O3'-C3'	-10.18	107.49	119.70
2	W	15	DT	P-O3'-C3'	-8.91	109.01	119.70
1	X	15	DC	P-O3'-C3'	-8.56	109.42	119.70
1	X	17	DG	P-O3'-C3'	-8.52	109.48	119.70
1	X	13	DA	P-O3'-C3'	-7.57	110.62	119.70
1	X	6	DA	P-O3'-C3'	-7.25	110.99	119.70
1	X	10	DA	P-O3'-C3'	-7.15	111.12	119.70
2	W	14	DT	P-O3'-C3'	-7.09	111.19	119.70
1	X	8	DT	O4'-C4'-C3'	-7.08	101.67	104.50
2	W	13	DT	P-O3'-C3'	-7.06	111.22	119.70
2	W	5	DA	P-O3'-C3'	-6.59	111.79	119.70
2	W	7	DA	O4'-C1'-N9	-6.19	103.67	108.00
2	W	8	DT	O4'-C1'-N1	-6.14	103.70	108.00
1	X	16	DA	OP1-P-O3'	6.12	118.68	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	9	DT	O4'-C1'-N1	6.01	112.21	108.00
2	W	10	DT	P-O3'-C3'	-6.00	112.50	119.70
2	W	9	DC	OP1-P-OP2	-5.98	110.62	119.60
1	X	23	DT	O4'-C1'-N1	-5.96	103.82	108.00
1	X	16	DA	P-O3'-C3'	-5.96	112.55	119.70
2	W	16	DT	P-O3'-C3'	-5.88	112.65	119.70
2	W	17	DA	C8-N9-C1'	5.65	137.87	127.70
2	W	17	DA	C4-N9-C1'	-5.59	116.24	126.30
1	X	2	DA	P-O3'-C3'	5.55	126.36	119.70
1	X	4	DG	O4'-C1'-N9	-5.54	104.12	108.00
2	W	14	DT	O4'-C1'-N1	-5.43	104.20	108.00
2	W	7	DA	P-O3'-C3'	-5.34	113.29	119.70
1	X	8	DT	OP1-P-O3'	5.27	116.80	105.20
1	X	20	DG	P-O3'-C3'	-5.23	113.42	119.70
2	W	20	DT	P-O3'-C3'	-5.22	113.43	119.70
1	X	11	DA	OP2-P-O3'	5.19	116.62	105.20
1	X	21	DT	P-O3'-C3'	-5.13	113.54	119.70
1	X	8	DT	C4'-C3'-C2'	-5.11	98.50	103.10
1	X	12	DA	OP2-P-O3'	5.11	116.44	105.20
2	W	24	DT	P-O3'-C3'	-5.11	113.57	119.70
2	W	9	DC	P-O3'-C3'	5.10	125.82	119.70
2	W	15	DT	OP2-P-O3'	5.05	116.32	105.20
1	X	4	DG	OP1-P-O3'	5.04	116.29	105.20

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	518	0	284	24	0
2	W	507	0	286	27	0
3	E	551	0	541	13	0
4	A	517	0	559	13	0
5	B	543	0	560	22	0
6	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	0	0	0
6	E	2	0	0	1	0
6	W	3	0	0	2	0
6	X	12	0	0	2	0
All	All	2663	0	2230	87	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 18.

All (87) 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:9:DT:H71	2:W:17:DA:N1	1.70	1.07
2:W:23:DC:H4'	2:W:24:DT:OP1	1.71	0.90
1:X:9:DT:C7	2:W:17:DA:N1	2.39	0.86
3:E:261:TRP:CH2	3:E:265:ARG:HG3	2.16	0.79
1:X:9:DT:C7	2:W:17:DA:C2	2.72	0.71
1:X:1:DA:H1'	1:X:2:DA:OP1	1.91	0.70
2:W:1:DA:N3	6:W:101:HOH:O	2.23	0.69
1:X:9:DT:H71	2:W:17:DA:C2	2.27	0.69
5:B:102:SER:HB3	5:B:105:GLU:HB3	1.78	0.65
1:X:8:DT:H2'	1:X:9:DT:C2	2.32	0.65
1:X:1:DA:H2	6:X:106:HOH:O	1.79	0.64
3:E:261:TRP:CZ2	3:E:265:ARG:HG3	2.33	0.63
2:W:11:DG:N3	6:W:102:HOH:O	2.31	0.61
3:E:240:ASP:O	3:E:243:ALA:HB3	2.02	0.60
4:A:565:ARG:HE	4:A:567:MET:HB3	1.67	0.59
1:X:19:DT:H6	5:B:110:ARG:HH22	1.50	0.59
5:B:110:ARG:NH2	5:B:114:ASN:HD21	2.01	0.58
4:A:610:ALA:O	4:A:614:ILE:HG23	2.02	0.58
3:E:238:TYR:CE2	5:B:142:LYS:HB2	2.38	0.58
4:A:614:ILE:HG22	5:B:156:ILE:HG12	1.85	0.57
3:E:254:THR:HG23	3:E:257:ARG:HG2	1.86	0.57
1:X:24:DT:C2'	1:X:25:DT:H72	2.36	0.56
5:B:146:ILE:HD12	5:B:146:ILE:H	1.71	0.56
4:A:572:ARG:O	4:A:573:GLU:HB3	2.05	0.55
1:X:5:DT:H4'	1:X:6:DA:OP1	2.06	0.55
4:A:589[B]:ARG:NH2	4:A:590:MET:SD	2.82	0.53
1:X:9:DT:H4'	1:X:10:DA:OP1	2.09	0.53
2:W:1:DA:H2"	2:W:2:DA:C8	2.44	0.52
2:W:1:DA:H3'	2:W:1:DA:OP2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:109:GLN:O	5:B:112:MET:HG2	2.10	0.52
3:E:216:ARG:O	3:E:217:ASN:HB3	2.09	0.51
2:W:24:DT:H1'	2:W:25:DT:H5"	1.93	0.51
2:W:24:DT:H2"	2:W:25:DT:H5'	1.93	0.51
1:X:3:DG:H2"	1:X:4:DG:OP2	2.10	0.50
1:X:8:DT:H2'	1:X:9:DT:O2	2.11	0.49
4:A:586:GLU:OE1	4:A:589[B]:ARG:HD3	2.12	0.49
5:B:124:LEU:C	5:B:125:ASN:O	2.51	0.49
5:B:138:LEU:HD12	5:B:140:SER:OG	2.13	0.49
4:A:571:ALA:O	4:A:574:ARG:HB2	2.13	0.49
5:B:141:ASP:O	5:B:142:LYS:HB3	2.13	0.48
3:E:277:GLN:NE2	6:E:302:HOH:O	2.46	0.48
3:E:268:LYS:O	3:E:271:LYS:HG3	2.15	0.47
3:E:234:GLN:NE2	3:E:234:GLN:HA	2.29	0.47
5:B:138:LEU:CD1	5:B:140:SER:OG	2.62	0.47
4:A:589[A]:ARG:HH12	4:A:601:GLN:HG3	1.80	0.47
5:B:138:LEU:HD12	5:B:140:SER:H	1.80	0.47
1:X:9:DT:C4'	1:X:10:DA:OP1	2.63	0.47
2:W:10:DT:H2"	2:W:11:DG:C8	2.51	0.46
1:X:5:DT:O2	3:E:218:ARG:NH2	2.32	0.46
2:W:1:DA:C3'	2:W:1:DA:P	3.04	0.46
5:B:131:LEU:O	5:B:132:ARG:HB2	2.16	0.45
5:B:166:ASP:O	5:B:167:GLU:C	2.53	0.45
1:X:9:DT:H72	2:W:17:DA:C2	2.52	0.45
1:X:9:DT:H2"	1:X:10:DA:C8	2.52	0.45
4:A:589[A]:ARG:HA	4:A:589[A]:ARG:HD3	1.71	0.45
3:E:271:LYS:HD3	3:E:277:GLN:HE22	1.82	0.45
2:W:24:DT:H1'	2:W:25:DT:C5'	2.47	0.44
2:W:1:DA:H3'	2:W:1:DA:P	2.58	0.44
2:W:2:DA:OP2	2:W:2:DA:H2'	2.18	0.44
2:W:16:DT:H2"	2:W:17:DA:C8	2.53	0.44
1:X:22:DG:H1'	1:X:23:DT:H5'	2.00	0.43
3:E:253:LEU:HD12	3:E:253:LEU:HA	1.86	0.43
3:E:264:ASN:O	3:E:267:ALA:HB3	2.19	0.43
1:X:18:DA:OP2	5:B:118:ARG:NH1	2.48	0.43
1:X:19:DT:H2'	5:B:110:ARG:NH2	2.33	0.43
2:W:1:DA:H4'	2:W:1:DA:OP1	2.19	0.43
2:W:23:DC:H2"	2:W:24:DT:H71	2.01	0.43
1:X:24:DT:H2'	1:X:25:DT:H72	2.01	0.43
1:X:1:DA:C1'	1:X:2:DA:OP1	2.65	0.43
2:W:21:DA:H2"	2:W:22:DC:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:22:DC:H1'	2:W:23:DC:C6	2.53	0.43
5:B:116:ARG:HD3	5:B:120:ARG:HH22	1.82	0.43
5:B:147:GLN:HE21	5:B:147:GLN:HB3	1.59	0.43
2:W:23:DC:C4'	2:W:24:DT:OP1	2.56	0.42
1:X:9:DT:H72	2:W:17:DA:N1	2.32	0.42
4:A:602:THR:O	4:A:606:ILE:HD12	2.20	0.42
2:W:7:DA:H1'	2:W:8:DT:H5'	2.01	0.42
5:B:132:ARG:NH2	5:B:143:LEU:O	2.52	0.42
5:B:124:LEU:HD13	5:B:124:LEU:HA	1.94	0.41
4:A:602:THR:HG22	4:A:605:LEU:H	1.85	0.41
2:W:8:DT:H2"	2:W:9:DC:H5'	2.03	0.41
1:X:2:DA:H1'	1:X:3:DG:H5'	2.03	0.41
4:A:595:LEU:O	4:A:595:LEU:HG	2.21	0.40
2:W:21:DA:H2"	2:W:22:DC:C5	2.56	0.40
6:X:112:HOH:O	5:B:110:ARG:HD2	2.21	0.40
5:B:107:GLN:O	5:B:110:ARG:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	E	60/62 (97%)	54 (90%)	4 (7%)	2 (3%)	4 15
4	A	60/60 (100%)	54 (90%)	3 (5%)	3 (5%)	2 7
5	B	64/67 (96%)	56 (88%)	8 (12%)	0	100 100
All	All	184/189 (97%)	164 (89%)	15 (8%)	5 (3%)	5 19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	601	GLN

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Mol	Chain	Res	Type
3	E	217	ASN
3	E	276	GLY
4	A	572	ARG
4	A	611	VAL

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
3	E	57/57 (100%)	45 (79%)	12 (21%)	1 3
4	A	56/54 (104%)	41 (73%)	15 (27%)	0 1
5	B	60/61 (98%)	46 (77%)	14 (23%)	1 2
All	All	173/172 (101%)	132 (76%)	41 (24%)	1 2

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	216	ARG
3	E	231	LYS
3	E	235	LYS
3	E	236	THR
3	E	250	ARG
3	E	253	LEU
3	E	254	THR
3	E	259	GLN
3	E	265	ARG
3	E	273	GLU
3	E	275	PHE
3	E	277	GLN
4	A	567	MET
4	A	578	ARG
4	A	580	ILE
4	A	589[A]	ARG
4	A	589[B]	ARG
4	A	595	LEU

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Mol	Chain	Res	Type
4	A	596	LYS
4	A	597	SER
4	A	599	LYS
4	A	602	THR
4	A	614	ILE
4	A	617	LEU
4	A	619	GLN
4	A	622	ARG
4	A	624	ARG
5	B	103	TYR
5	B	104	GLU
5	B	107	GLN
5	B	109	GLN
5	B	111	VAL
5	B	112	MET
5	B	119	GLN
5	B	124	LEU
5	B	135	ILE
5	B	140	SER
5	B	146	ILE
5	B	147	GLN
5	B	150	LYS
5	B	167	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	225	GLN
3	E	234	GLN
3	E	263	GLN
3	E	264	ASN
3	E	277	GLN
4	A	594	HIS
4	A	619	GLN
5	B	114	ASN
5	B	119	GLN
5	B	147	GLN

5.3.3 RNA

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 monosaccharides 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, 95^{th} 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	25/25 (100%)	-0.27	0	100	100	64, 85, 112, 120	0
2	W	25/25 (100%)	-0.31	0	100	100	68, 77, 102, 122	0
3	E	62/62 (100%)	0.29	4 (6%)	18	14	60, 105, 139, 144	0
4	A	60/60 (100%)	0.28	1 (1%)	70	69	62, 85, 135, 157	0
5	B	66/67 (98%)	0.37	2 (3%)	50	45	57, 88, 148, 186	0
All	All	238/239 (99%)	0.19	7 (2%)	51	47	57, 90, 139, 186	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	217	ASN	2.4
3	E	277	GLN	2.3
5	B	167	GLU	2.3
3	E	271	LYS	2.3
4	A	571	ALA	2.2
5	B	107	GLN	2.0
3	E	275	PHE	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

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.