Full wwPDB X-ray Structure Validation Report Ⓘ

Feb 1, 2016 – 10:13 PM GMT

PDB ID	:	4X3U
Title	:	Crystal structure of chromobox homolog 7 (CBX7) chromodomain with Suramin
Authors	:	Ren, C.; Zhou, M.M.
Deposited on	:	2014-12-01
Resolution	:	1.63 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 1.63 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		1.0%
RSRZ outliers		7.3%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
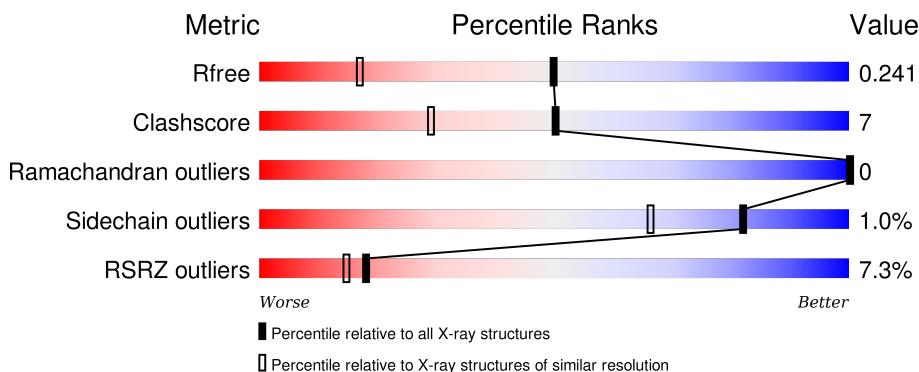
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

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	A	64	3% / 80% / 6% · 13%
1	B	64	9% / 70% / 11% · 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1267 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 Chromobox protein homolog 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	0	0
			487	315	87	84	1			
1	B	53	Total	C	N	O	S	0	0	0
			459	301	78	79	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP Q8VDS3
A	4	SER	-	expression tag	UNP Q8VDS3
A	5	HIS	-	expression tag	UNP Q8VDS3
A	6	MET	-	expression tag	UNP Q8VDS3
B	3	GLY	-	expression tag	UNP Q8VDS3
B	4	SER	-	expression tag	UNP Q8VDS3
B	5	HIS	-	expression tag	UNP Q8VDS3
B	6	MET	-	expression tag	UNP Q8VDS3

- Molecule 2 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: $C_{51}H_{40}N_6O_{23}S_6$).
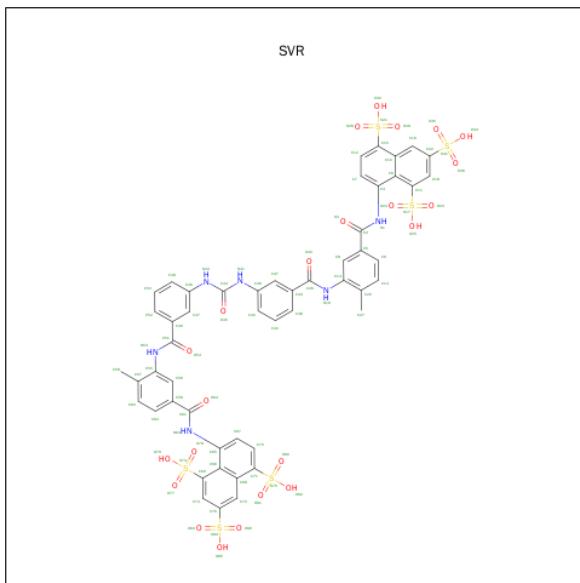
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	B	1	Total	C	N	O	S	0	0
			86	51	6	23	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	67	Total	O	0	0
			67	67		

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: Chromobox protein homolog 7

Chain A:

- Molecule 1: Chromobox protein homolog 7

Chain B:
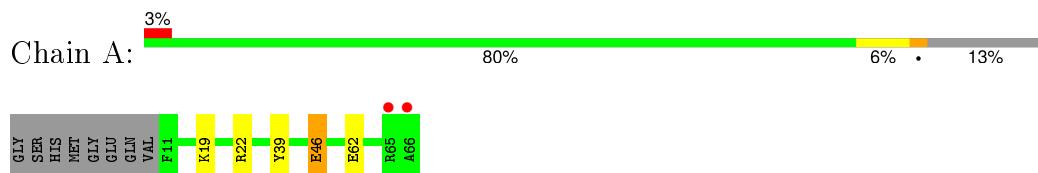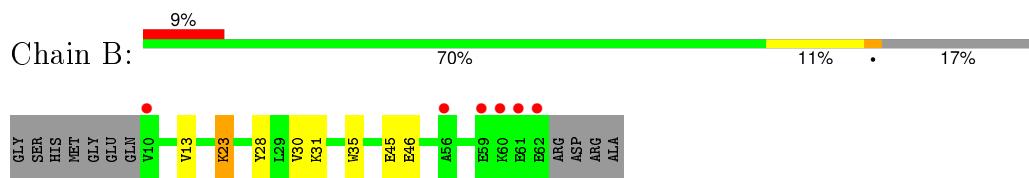
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	58.70Å 58.70Å 89.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.68 – 1.63 22.67 – 1.63	Depositor EDS
% Data completeness (in resolution range)	98.8 (22.68-1.63) 98.8 (22.67-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.16 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.160 , 0.232 0.173 , 0.241	Depositor DCC
R_{free} test set	1016 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 71.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\vert L\vert> = 0.47$, $<L^2> = 0.30$	Xtriage
Outliers	0 of 19972 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	1267	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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 $<\vert L\vert>$, $<L^2>$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: SVR

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	1.34	5/501 (1.0%)	1.14	2/673 (0.3%)
1	B	1.18	3/473 (0.6%)	1.15	1/637 (0.2%)
All	All	1.27	8/974 (0.8%)	1.14	3/1310 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	GLU	CD-OE1	8.32	1.34	1.25
1	A	62	GLU	CD-OE1	6.26	1.32	1.25
1	B	28	TYR	CE1-CZ	-5.69	1.31	1.38
1	A	39	TYR	CE1-CZ	-5.55	1.31	1.38
1	B	35	TRP	CG-CD1	-5.46	1.29	1.36
1	A	39	TYR	CG-CD2	-5.39	1.32	1.39
1	B	35	TRP	CB-CG	-5.39	1.40	1.50
1	A	62	GLU	CG-CD	5.36	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	LYS	CD-CE-NZ	7.86	129.77	111.70
1	A	62	GLU	OE1-CD-OE2	-6.10	115.98	123.30
1	A	62	GLU	CG-CD-OE1	5.79	129.87	118.30

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	A	487	0	491	3	0
1	B	459	0	465	6	0
2	B	172	0	78	7	0
3	A	82	0	0	2	0
3	B	67	0	0	3	0
All	All	1267	0	1034	15	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 7.

All (15) 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:B:13:VAL:HG13	1:B:30:VAL:HG13	1.71	0.72
1:A:22:ARG:NH1	1:B:23:LYS:HE3	2.08	0.68
1:B:46:GLU:OE1	3:B:201:HOH:O	2.11	0.67
2:B:102:SVR:S17	2:B:102:SVR:N1	2.73	0.61
2:B:101:SVR:S17	2:B:101:SVR:N1	2.81	0.53
1:B:45:GLU:HB2	3:B:253:HOH:O	2.10	0.52
2:B:102:SVR:O45	2:B:102:SVR:H47	2.13	0.49
1:A:46:GLU:OE1	3:A:102:HOH:O	2.20	0.48
2:B:101:SVR:C26	2:B:101:SVR:H271	2.44	0.47
2:B:102:SVR:H593	2:B:102:SVR:O54	2.15	0.47
1:A:19:LYS:NZ	3:A:105:HOH:O	2.43	0.46
2:B:102:SVR:S73	2:B:102:SVR:N63	2.89	0.44
1:B:45:GLU:CB	3:B:253:HOH:O	2.65	0.44
2:B:102:SVR:O4	2:B:102:SVR:H7	2.17	0.43
1:B:23:LYS:CG	1:B:23:LYS:O	2.68	0.41

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	
1	A	54/64 (84%)	54 (100%)	0	0	100	100
1	B	51/64 (80%)	51 (100%)	0	0	100	100
All	All	105/128 (82%)	105 (100%)	0	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	51/57 (90%)	51 (100%)	0	100	100
1	B	49/57 (86%)	48 (98%)	1 (2%)	63	35
All	All	100/114 (88%)	99 (99%)	1 (1%)	82	66

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	SVR	B	101	-	93,93,93	2.68	33 (35%)	133,145,145	2.88	33 (24%)
2	SVR	B	102	-	93,93,93	3.07	34 (36%)	133,145,145	3.06	47 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SVR	B	101	-	-	0/76/76/76	0/8/8/8
2	SVR	B	102	-	-	0/76/76/76	0/8/8/8

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	SVR	C15-S21	-11.45	1.61	1.78
2	B	101	SVR	C11-S17	-11.33	1.61	1.78
2	B	102	SVR	C11-S17	-9.18	1.64	1.78
2	B	101	SVR	C15-S21	-9.11	1.64	1.78
2	B	101	SVR	C76-S83	-7.92	1.61	1.76
2	B	102	SVR	C76-S83	-7.91	1.61	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	SVR	C71-S75	-7.84	1.66	1.78
2	B	101	SVR	C71-S75	-7.21	1.67	1.78
2	B	102	SVR	C69-S73	-7.11	1.67	1.78
2	B	102	SVR	C22-S31	-5.52	1.66	1.76
2	B	101	SVR	C69-S73	-3.84	1.72	1.78
2	B	102	SVR	C13-N19	-3.30	1.35	1.41
2	B	101	SVR	O78-S73	-3.29	1.27	1.43
2	B	102	SVR	C39-N41	-3.21	1.35	1.41
2	B	101	SVR	C22-S31	-3.19	1.70	1.76
2	B	102	SVR	C55-N53	-3.13	1.35	1.41
2	B	101	SVR	C46-N44	-3.05	1.35	1.41
2	B	101	SVR	C42-C39	-2.73	1.34	1.39
2	B	101	SVR	C43-N41	-2.29	1.33	1.37
2	B	101	SVR	O80-S75	-2.24	1.32	1.43
2	B	101	SVR	C55-N53	-2.21	1.37	1.41
2	B	101	SVR	C13-N19	-2.17	1.37	1.41
2	B	101	SVR	O84-S83	-2.09	1.33	1.43
2	B	102	SVR	C33-C26	2.00	1.54	1.50
2	B	101	SVR	C74-C76	2.00	1.42	1.39
2	B	101	SVR	C71-C68	2.06	1.46	1.43
2	B	102	SVR	O85-S83	2.14	1.56	1.44
2	B	102	SVR	C12-C15	2.16	1.40	1.37
2	B	101	SVR	C12-C15	2.18	1.40	1.37
2	B	102	SVR	C7-C3	2.19	1.43	1.38
2	B	101	SVR	C56-C58	2.23	1.42	1.39
2	B	101	SVR	C50-C48	2.24	1.43	1.38
2	B	102	SVR	O4-C2	2.27	1.27	1.23
2	B	101	SVR	C10-C6	2.37	1.47	1.42
2	B	101	SVR	C15-C10	2.43	1.47	1.43
2	B	101	SVR	C9-C5	2.46	1.43	1.39
2	B	101	SVR	O4-C2	2.51	1.28	1.23
2	B	102	SVR	C5-C2	2.64	1.55	1.50
2	B	102	SVR	C52-C49	2.70	1.43	1.39
2	B	101	SVR	C65-C66	2.71	1.46	1.42
2	B	102	SVR	C65-C66	2.82	1.47	1.42
2	B	102	SVR	C16-C22	2.85	1.41	1.36
2	B	102	SVR	C18-C11	2.87	1.41	1.37
2	B	101	SVR	O34-S31	2.93	1.60	1.44
2	B	102	SVR	C38-C33	3.00	1.44	1.39
2	B	101	SVR	C40-C42	3.18	1.45	1.38
2	B	101	SVR	O64-C61	3.31	1.30	1.23
2	B	102	SVR	O25-S17	3.36	1.63	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	SVR	O82-S75	3.38	1.63	1.44
2	B	102	SVR	C71-C68	3.43	1.48	1.43
2	B	102	SVR	C10-C6	3.53	1.49	1.42
2	B	101	SVR	C68-C66	3.59	1.49	1.42
2	B	101	SVR	C3-C6	3.60	1.48	1.42
2	B	102	SVR	O30-S21	3.77	1.65	1.44
2	B	101	SVR	O25-S17	3.78	1.65	1.44
2	B	102	SVR	C68-C66	4.09	1.50	1.42
2	B	102	SVR	C15-C10	4.11	1.49	1.43
2	B	102	SVR	O79-S73	4.15	1.67	1.44
2	B	102	SVR	O34-S31	4.21	1.67	1.44
2	B	101	SVR	C13-C20	4.73	1.49	1.40
2	B	102	SVR	C13-C20	4.75	1.49	1.40
2	B	101	SVR	C69-C66	4.85	1.50	1.43
2	B	102	SVR	C11-C6	5.02	1.50	1.43
2	B	101	SVR	C11-C6	5.93	1.52	1.43
2	B	102	SVR	C69-C66	6.05	1.52	1.43
2	B	102	SVR	C55-C57	6.37	1.52	1.40
2	B	102	SVR	C3-C6	6.60	1.52	1.42

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	101	SVR	O64-C61-C58	-8.94	105.69	120.97
2	B	102	SVR	O35-S31-C22	-8.32	86.22	106.63
2	B	102	SVR	O36-S31-C22	-7.75	87.62	106.63
2	B	101	SVR	O78-S73-C69	-7.08	98.17	106.20
2	B	102	SVR	C70-C71-C68	-6.20	115.52	121.04
2	B	101	SVR	O25-S17-O24	-5.94	80.12	111.64
2	B	101	SVR	O36-S31-C22	-5.90	92.16	106.63
2	B	102	SVR	C74-C76-S83	-5.78	109.57	119.97
2	B	102	SVR	O25-S17-O24	-5.00	85.10	111.64
2	B	102	SVR	C74-C69-C66	-4.90	113.96	120.80
2	B	102	SVR	C67-C65-C66	-4.81	114.61	120.30
2	B	102	SVR	O34-S31-C22	-4.75	93.52	106.94
2	B	102	SVR	O30-S21-O28	-4.74	86.47	111.64
2	B	102	SVR	O85-S83-O84	-4.45	88.03	111.64
2	B	102	SVR	O25-S17-O23	-4.31	88.78	111.64
2	B	101	SVR	O4-C2-C5	-3.64	114.76	120.97
2	B	101	SVR	C62-C58-C56	-3.57	114.92	119.24
2	B	101	SVR	C18-C11-C6	-3.52	115.89	120.80
2	B	102	SVR	C56-C55-N53	-3.50	112.78	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	SVR	C65-N63-C61	-3.48	117.90	128.87
2	B	102	SVR	O30-S21-O29	-3.38	93.72	111.64
2	B	102	SVR	O84-S83-O86	-3.28	94.75	112.46
2	B	102	SVR	C72-C68-C71	-3.15	119.60	123.23
2	B	102	SVR	C59-C57-C60	-2.99	114.23	120.33
2	B	102	SVR	C27-C20-C13	-2.97	118.27	121.36
2	B	102	SVR	O64-C61-C58	-2.94	115.94	120.97
2	B	102	SVR	C7-C3-C6	-2.80	116.98	120.30
2	B	101	SVR	C8-C13-C20	-2.66	116.96	120.01
2	B	101	SVR	C74-C69-C66	-2.56	117.23	120.80
2	B	101	SVR	C74-C76-S83	-2.43	115.59	119.97
2	B	102	SVR	C12-C15-C10	-2.36	118.94	121.04
2	B	101	SVR	O35-S31-C22	-2.10	101.47	106.63
2	B	101	SVR	O34-S31-C22	-2.03	101.20	106.94
2	B	101	SVR	C5-C2-N1	2.06	119.96	115.94
2	B	101	SVR	C39-N41-C43	2.15	130.80	126.65
2	B	102	SVR	C42-C39-C37	2.16	122.27	119.69
2	B	101	SVR	C76-C74-C69	2.17	122.37	120.09
2	B	101	SVR	C62-C58-C61	2.17	127.48	120.60
2	B	102	SVR	O85-S83-O86	2.20	123.32	111.64
2	B	101	SVR	C42-C39-C37	2.21	122.33	119.69
2	B	101	SVR	C57-C55-N53	2.24	122.21	118.71
2	B	101	SVR	C60-C62-C58	2.28	123.41	120.76
2	B	102	SVR	O24-S17-O23	2.29	124.82	112.46
2	B	102	SVR	C60-C57-C55	2.39	119.27	117.39
2	B	102	SVR	C39-N41-C43	2.39	131.27	126.65
2	B	102	SVR	C67-C70-C71	2.46	124.65	121.77
2	B	102	SVR	C70-C67-C65	2.55	125.14	120.67
2	B	102	SVR	C14-C20-C13	2.55	119.39	117.39
2	B	101	SVR	C40-C38-C33	2.56	123.55	120.33
2	B	102	SVR	O29-S21-O28	2.57	126.31	112.46
2	B	101	SVR	C14-C20-C13	2.73	119.54	117.39
2	B	102	SVR	O78-S73-C69	2.75	109.32	106.20
2	B	101	SVR	O64-C61-N63	2.77	129.77	123.68
2	B	101	SVR	O85-S83-C76	2.88	115.06	106.94
2	B	102	SVR	O80-S75-C71	3.00	109.61	106.20
2	B	102	SVR	C69-C66-C68	3.02	119.34	116.31
2	B	102	SVR	C22-C18-C11	3.02	123.27	120.09
2	B	102	SVR	O85-S83-C76	3.07	115.59	106.94
2	B	102	SVR	C70-C71-S75	3.17	122.18	117.51
2	B	101	SVR	C18-C11-S17	3.22	123.40	117.82
2	B	101	SVR	O86-S83-C76	3.53	115.29	106.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	SVR	C11-C6-C10	3.75	120.07	116.31
2	B	101	SVR	C22-C18-C11	3.78	124.06	120.09
2	B	102	SVR	C18-C11-S17	3.83	124.46	117.82
2	B	101	SVR	O34-S31-O36	4.28	134.34	111.64
2	B	101	SVR	C58-C61-N63	4.32	124.36	115.94
2	B	102	SVR	O86-S83-C76	4.51	117.70	106.63
2	B	102	SVR	C72-C76-S83	4.69	128.39	119.96
2	B	102	SVR	C59-C57-C55	4.92	126.49	121.36
2	B	102	SVR	O77-S73-C69	5.02	111.89	106.20
2	B	102	SVR	C12-C15-S21	5.40	125.47	117.51
2	B	102	SVR	C76-C74-C69	5.64	126.03	120.09
2	B	102	SVR	C57-C55-N53	5.96	128.01	118.71
2	B	102	SVR	O29-S21-C15	6.43	113.49	106.20
2	B	101	SVR	O77-S73-C69	6.58	113.66	106.20
2	B	102	SVR	O23-S17-C11	7.11	114.26	106.20
2	B	101	SVR	O28-S21-C15	7.62	114.83	106.20
2	B	102	SVR	O28-S21-C15	11.56	119.30	106.20
2	B	102	SVR	O24-S17-C11	12.93	120.86	106.20
2	B	101	SVR	O23-S17-C11	21.64	130.73	106.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	101	SVR	2	0
2	B	102	SVR	5	0

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	A	56/64 (87%)	-0.17	2 (3%)	46	44	5, 15, 28, 33	0
1	B	53/64 (82%)	0.52	6 (11%)	7	5	5, 20, 63, 77	0
All	All	109/128 (85%)	0.17	8 (7%)	18	15	5, 17, 42, 77	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	GLU	4.6
1	B	62	GLU	4.6
1	B	61	GLU	3.8
1	B	10	VAL	3.5
1	A	66	ALA	2.6
1	B	60	LYS	2.3
1	A	65	ARG	2.2
1	B	56	ALA	2.2

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SVR	B	102	86/86	0.95	0.16	0.69	11,24,59,77	0
2	SVR	B	101	86/86	0.98	0.08	-0.63	3,7,27,29	0

6.5 Other polymers (i)

There are no such residues in this entry.