



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6Q8F / pdb_00006q8f
Title : Nterminal domain of human SMU1
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Deposited on : 2018-12-14
Resolution : 1.90 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

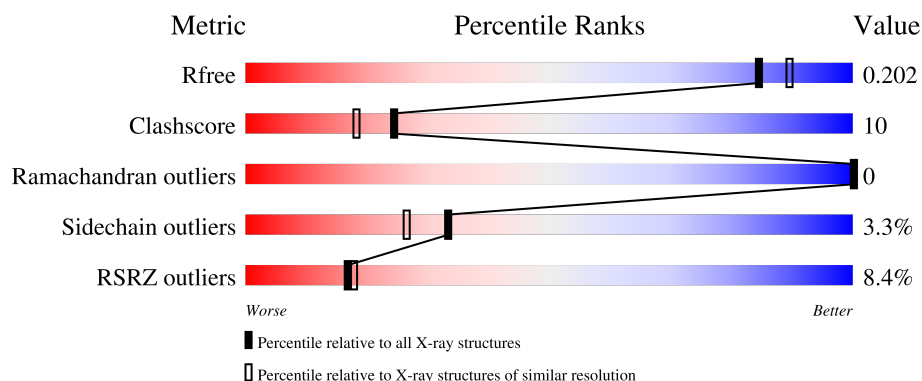
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	514	 3% 31% 6% 60%
1	B	514	 3% 31% 6% 60%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3260 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.

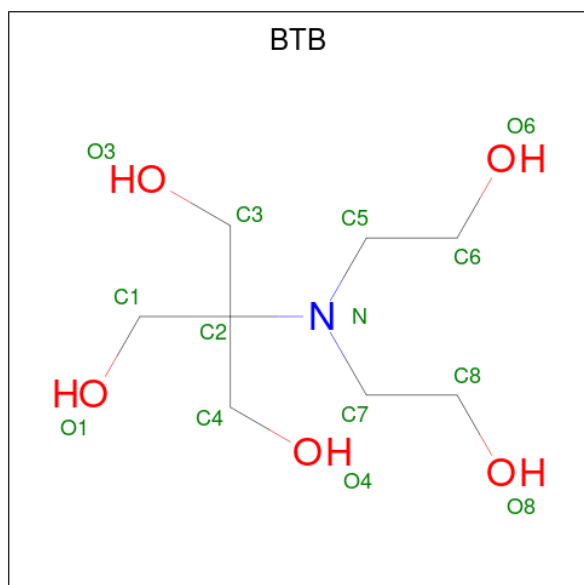
- Molecule 1 is a protein called WD40 repeat-containing protein SMU1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	1	0
			1564	994	270	295	5			
1	B	184	Total	C	N	O	S	0	0	0
			1464	928	254	278	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q2TAY7
A	1	GLY	-	expression tag	UNP Q2TAY7
B	0	MET	-	initiating methionine	UNP Q2TAY7
B	1	GLY	-	expression tag	UNP Q2TAY7

- Molecule 2 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	103	Total	O	0	0
			103	103		

MET	GLY
LYS	LYS
THR	THR
THR	THR
GLY	GLY
CYS	GLY
SER	SER
ASN	ASN
PHE	PHE
THR	THR
CYS	CYS
LYS	LYS
SER	SER
LEU	LEU
GLY	GLY
THR	THR
ASP	ASP
ILE	ILE
THR	THR
THR	THR
VAL	VAL
ASN	GLY
SER	SER
VAL	ASP
ILE	PHE
LEU	VAL
LEU	LEU
PRO	TYR
LYS	CYS
ASN	PHE
PRO	THR
GLU	VAL
THR	HIS
GLU	THR
ASN	THR
VAL	GLY
CYS	LYS
ASN	VAL
THR	VAL
THR	CYS
VAL	LEU
VAL	GLU
ILE	ASN
MET	ARG
ASN	THR
MET	SER
GLN	ASN
GLY	THR
GLN	VAL
ILE	HIS
ALA	VAL
HIS	ARG
HIS	SER
PRO	THR
HIS	PHE
GLN	SER
ASN	ASN

GLY
LYS
ARG
THR
GLU
TYR
SER
GLU
ASP
PHE
VAL
THR
CYS
LYS
ALA
SER
LEU
LEU
SER
GLY
PRO
THR
ARG
GLY
GLY
TRP
THR
ASP
ILE
TYR
CYS
VAL
VAL
GLY
SER
GLU
ASP
VAL
PHE
VAL
LEU
LEU
TYR
PRO
CYS
PHE
SER
THR
VAL
THR
THR
GLY
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GLU
ASN
ARG
THR
THR
LEU
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ASN
VAL
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GLY
GLN
ILE
ALA
ILE
HIS
VAL
ARG
SER
THR
PHE
SER
GLN
ASN

LEU
ILE
ALA
THR
GLU
TYR
SER
GLU
ASP
PHE
VAL
THR
CYS
LYS
ALA
SER
LEU
LEU
SER
GLY
PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.18Å 41.23Å 123.60Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	39.14 – 1.90 39.14 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.14-1.90) 97.2 (39.14-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.174 , 0.214 (Not available) , 0.202	Depositor DCC
R_{free} test set	1610 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l 0.024 for k,h,-l 0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3260	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.96% 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

5.1 Standard geometry

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

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	0.98	0/1592	1.35	4/2156 (0.2%)
1	B	0.98	0/1486	1.33	0/2012
All	All	0.98	0/3078	1.34	4/4168 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	23	LEU	CA-C-N	5.11	127.08	120.44
1	A	23	LEU	C-N-CA	5.11	127.08	120.44
1	A	193	VAL	CA-C-N	5.08	128.44	120.82
1	A	193	VAL	C-N-CA	5.08	128.44	120.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	PRO	Peptide
1	B	65	SER	Peptide

5.2 Too-close contacts ⓘ

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	1564	0	1609	32	0
1	B	1464	0	1495	36	0
2	A	14	0	19	3	0
3	B	1	0	0	1	0
4	A	114	0	0	2	0
4	B	103	0	0	0	0
All	All	3260	0	3123	61	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 10.

All (61) 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:A:601:BTB:O4	2:A:601:BTB:H71	1.68	0.92
1:A:107:LYS:HD2	4:A:790:HOH:O	1.73	0.89
1:B:40:THR:HB	1:B:43:SER:HB2	1.53	0.87
1:B:65:SER:HB2	1:B:66:LEU:HD23	1.55	0.87
1:A:40:THR:HG23	1:B:41:VAL:CG2	2.05	0.86
1:A:15:MET:CE	1:A:31:GLN:HA	2.07	0.83
1:A:41:VAL:HG13	1:B:41:VAL:HG13	1.61	0.83
1:B:35:THR:C	1:B:36:VAL:N	2.40	0.78
1:B:41:VAL:HA	1:B:44:ILE:HG22	1.64	0.78
1:A:15:MET:HE1	1:A:31:GLN:HA	1.67	0.75
1:A:41:VAL:HG21	1:B:40:THR:HA	1.68	0.74
1:A:3:ILE:HD12	1:A:3:ILE:O	1.88	0.73
1:A:40:THR:HA	1:B:41:VAL:HG21	1.78	0.66
1:B:3:ILE:HD12	1:B:3:ILE:O	1.95	0.66
1:B:35:THR:CA	1:B:36:VAL:N	2.59	0.65
1:A:15:MET:HE2	1:A:31:GLN:HA	1.79	0.62
1:B:185:ASP:OD1	1:B:188:ARG:HB2	2.01	0.60
1:B:40:THR:CB	1:B:43:SER:HB2	2.30	0.58
1:B:61:GLN:HA	1:B:64:GLN:HG2	1.85	0.57
1:A:52:ASN:HD21	1:A:143:ALA:HA	1.69	0.57
1:A:64:GLN:HG3	4:A:729:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:MET:HE2	1:A:31:GLN:CA	2.38	0.54
1:B:120:LEU:HD21	1:B:130:GLU:HB3	1.89	0.53
1:B:103:MET:HE2	1:B:103:MET:HA	1.90	0.52
1:A:103:MET:HA	1:A:103:MET:HE2	1.91	0.52
1:A:41:VAL:HG23	1:A:42:ASP:N	2.25	0.52
1:B:41:VAL:CA	1:B:44:ILE:HG22	2.37	0.52
1:A:40:THR:HG23	1:B:41:VAL:HG21	1.91	0.51
1:B:66:LEU:HB2	1:B:68:LEU:HG	1.93	0.51
1:B:66:LEU:O	1:B:67:LYS:C	2.54	0.51
1:A:112:GLU:O	1:A:115:ILE:HG22	2.12	0.49
1:B:65:SER:HB2	1:B:66:LEU:CD2	2.37	0.49
1:A:96:LEU:HD12	1:A:100:THR:HG21	1.94	0.49
1:B:61:GLN:HA	1:B:64:GLN:CG	2.42	0.49
1:A:116:HIS:CE1	1:A:120:LEU:HD11	2.48	0.48
1:B:35:THR:O	1:B:36:VAL:N	2.46	0.48
1:A:40:THR:HG23	1:B:41:VAL:HG23	1.90	0.47
1:B:12:ARG:HB3	1:B:38:LEU:CD2	2.45	0.47
1:A:45:GLU:OE1	1:B:20:GLU:OE2	2.33	0.46
1:A:60:LEU:O	1:A:63:ILE:HG13	2.16	0.45
1:B:41:VAL:O	1:B:44:ILE:HG22	2.17	0.45
1:B:66:LEU:HD23	1:B:66:LEU:N	2.31	0.45
2:A:601:BTB:O4	2:A:601:BTB:C7	2.54	0.45
1:B:40:THR:HB	1:B:43:SER:CB	2.38	0.44
1:A:41:VAL:O	1:A:45:GLU:HG2	2.17	0.44
1:B:35:THR:N	1:B:36:VAL:N	2.66	0.44
1:B:12:ARG:O	1:B:38:LEU:HD21	2.18	0.43
1:A:27:LEU:O	1:A:31:GLN:HG3	2.18	0.42
1:A:40:THR:CA	1:B:41:VAL:HG21	2.47	0.42
1:A:41:VAL:H	1:B:41:VAL:HG22	1.85	0.42
1:A:169:LEU:HD21	1:A:186:LEU:HD23	2.02	0.42
1:A:72[B]:THR:CG2	1:A:152:GLU:HG3	2.49	0.42
1:A:147:GLN:NE2	1:B:163:ALA:HB2	2.35	0.42
2:A:601:BTB:O6	2:A:601:BTB:H72	2.20	0.42
1:B:12:ARG:CB	1:B:38:LEU:HD23	2.50	0.42
1:A:41:VAL:CG2	1:A:42:ASP:N	2.83	0.41
1:B:171:TRP:NE1	3:B:601:CL:CL	2.86	0.41
1:A:12:ARG:HB3	1:A:38:LEU:HD21	2.03	0.41
1:B:12:ARG:HB3	1:B:38:LEU:HD23	2.03	0.41
1:A:101:ASP:N	1:A:102:PRO:CD	2.84	0.41
1:A:178:LEU:HA	1:A:179:PRO:HD3	1.93	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	194/514 (38%)	189 (97%)	5 (3%)	0	100	100
1	B	178/514 (35%)	177 (99%)	1 (1%)	0	100	100
All	All	372/1028 (36%)	366 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	173/450 (38%)	168 (97%)	5 (3%)	37	31
1	B	162/450 (36%)	155 (96%)	7 (4%)	26	18
All	All	335/900 (37%)	323 (96%)	12 (4%)	33	23

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	65	SER
1	A	72[A]	THR
1	A	72[B]	THR
1	A	200	LYS
1	B	35	THR
1	B	40	THR
1	B	43	SER

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Mol	Chain	Res	Type
1	B	65	SER
1	B	66	LEU
1	B	154	SER
1	B	185	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	52	ASN
1	A	119	ASN
1	A	147	GLN
1	B	24	HIS
1	B	55	HIS
1	B	99	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	BTB	A	601	-	13,13,13	1.42	2 (15%)	7,16,16	0.62	0

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	BTB	A	601	-	-	6/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BTB	C2-N	3.70	1.55	1.48
2	A	601	BTB	C5-N	2.73	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BTB	C1-C2-C4-O4
2	A	601	BTB	C1-C2-N-C7
2	A	601	BTB	C3-C2-N-C7
2	A	601	BTB	C4-C2-N-C7
2	A	601	BTB	C6-C5-N-C7
2	A	601	BTB	O1-C1-C2-C4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	BTB	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	35:THR	C	36:VAL	N	2.40

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	197/514 (38%)	0.12	17 (8%)	16 17	12, 22, 59, 80	1 (0%)
1	B	184/514 (35%)	0.22	15 (8%)	17 18	13, 24, 54, 109	0
All	All	381/1028 (37%)	0.17	32 (8%)	17 18	12, 23, 58, 109	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	VAL	6.5
1	B	184	ILE	5.9
1	B	40	THR	5.6
1	B	38	LEU	5.2
1	B	35	THR	4.1
1	B	64	GLN	4.1
1	B	39	ASN	3.9
1	A	196	VAL	3.8
1	A	64	GLN	3.8
1	A	180	PRO	3.6
1	B	180	PRO	3.5
1	A	193	VAL	3.5
1	B	3	ILE	3.1
1	B	179	PRO	2.9
1	A	66	LEU	2.9
1	A	3	ILE	2.8
1	A	182	MET	2.8
1	B	42	ASP	2.7
1	A	155	VAL	2.7
1	A	184	ILE	2.6
1	A	181	GLY	2.6
1	B	65	SER	2.6
1	A	179	PRO	2.5
1	A	183	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	40	THR	2.5
1	B	63	ILE	2.4
1	B	155	VAL	2.4
1	A	38	LEU	2.4
1	A	194	LYS	2.3
1	B	43	SER	2.3
1	A	41	VAL	2.3
1	A	39	ASN	2.1

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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	BTB	A	601	14/14	0.92	0.09	15,20,30,31	0
3	CL	B	601	1/1	0.96	0.08	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.