



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:38 AM UTC

PDB ID : 3OC3 / pdb_00003oc3
Title : Crystal structure of the Mot1 N-terminal domain in complex with TBP
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Hopfner, K.-P.
Deposited on : 2010-08-09
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

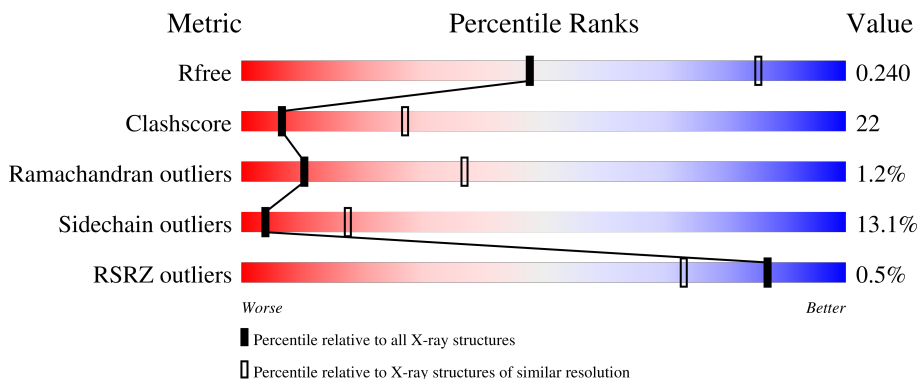
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	800	
1	B	800	
2	C	218	
2	D	218	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15037 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 HELICASE MOT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	752	6086	3926	984	1153	23	104	0	0
1	B	749	6064	3911	981	1149	23	72	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q8SVZ5
A	-20	ALA	-	expression tag	UNP Q8SVZ5
A	-19	HIS	-	expression tag	UNP Q8SVZ5
A	-18	HIS	-	expression tag	UNP Q8SVZ5
A	-17	HIS	-	expression tag	UNP Q8SVZ5
A	-16	HIS	-	expression tag	UNP Q8SVZ5
A	-15	HIS	-	expression tag	UNP Q8SVZ5
A	-14	HIS	-	expression tag	UNP Q8SVZ5
A	-13	HIS	-	expression tag	UNP Q8SVZ5
A	-12	HIS	-	expression tag	UNP Q8SVZ5
A	-11	HIS	-	expression tag	UNP Q8SVZ5
A	-10	HIS	-	expression tag	UNP Q8SVZ5
A	-9	ALA	-	expression tag	UNP Q8SVZ5
A	-8	GLY	-	expression tag	UNP Q8SVZ5
A	-7	ALA	-	expression tag	UNP Q8SVZ5
A	-6	GLY	-	expression tag	UNP Q8SVZ5
A	-5	ALA	-	expression tag	UNP Q8SVZ5
A	-4	ARG	-	expression tag	UNP Q8SVZ5
A	-3	ASN	-	expression tag	UNP Q8SVZ5
A	-2	MET	-	expression tag	UNP Q8SVZ5
A	-1	ALA	-	expression tag	UNP Q8SVZ5
A	0	SER	-	expression tag	UNP Q8SVZ5
B	-21	MET	-	expression tag	UNP Q8SVZ5
B	-20	ALA	-	expression tag	UNP Q8SVZ5
B	-19	HIS	-	expression tag	UNP Q8SVZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q8SVZ5
B	-17	HIS	-	expression tag	UNP Q8SVZ5
B	-16	HIS	-	expression tag	UNP Q8SVZ5
B	-15	HIS	-	expression tag	UNP Q8SVZ5
B	-14	HIS	-	expression tag	UNP Q8SVZ5
B	-13	HIS	-	expression tag	UNP Q8SVZ5
B	-12	HIS	-	expression tag	UNP Q8SVZ5
B	-11	HIS	-	expression tag	UNP Q8SVZ5
B	-10	HIS	-	expression tag	UNP Q8SVZ5
B	-9	ALA	-	expression tag	UNP Q8SVZ5
B	-8	GLY	-	expression tag	UNP Q8SVZ5
B	-7	ALA	-	expression tag	UNP Q8SVZ5
B	-6	GLY	-	expression tag	UNP Q8SVZ5
B	-5	ALA	-	expression tag	UNP Q8SVZ5
B	-4	ARG	-	expression tag	UNP Q8SVZ5
B	-3	ASN	-	expression tag	UNP Q8SVZ5
B	-2	MET	-	expression tag	UNP Q8SVZ5
B	-1	ALA	-	expression tag	UNP Q8SVZ5
B	0	SER	-	expression tag	UNP Q8SVZ5

- Molecule 2 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID (TFIID-1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	178	1417	919	247	244	7	8	1	0
2	D	178	1417	919	247	244	7	6	1	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP Q8ST28
C	-18	GLY	-	expression tag	UNP Q8ST28
C	-17	SER	-	expression tag	UNP Q8ST28
C	-16	SER	-	expression tag	UNP Q8ST28
C	-15	HIS	-	expression tag	UNP Q8ST28
C	-14	HIS	-	expression tag	UNP Q8ST28
C	-13	HIS	-	expression tag	UNP Q8ST28
C	-12	HIS	-	expression tag	UNP Q8ST28
C	-11	HIS	-	expression tag	UNP Q8ST28
C	-10	HIS	-	expression tag	UNP Q8ST28
C	-9	SER	-	expression tag	UNP Q8ST28

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP Q8ST28
C	-7	GLY	-	expression tag	UNP Q8ST28
C	-6	LEU	-	expression tag	UNP Q8ST28
C	-5	VAL	-	expression tag	UNP Q8ST28
C	-4	PRO	-	expression tag	UNP Q8ST28
C	-3	ARG	-	expression tag	UNP Q8ST28
C	-2	GLY	-	expression tag	UNP Q8ST28
C	-1	SER	-	expression tag	UNP Q8ST28
C	0	HIS	-	expression tag	UNP Q8ST28
D	-19	MET	-	expression tag	UNP Q8ST28
D	-18	GLY	-	expression tag	UNP Q8ST28
D	-17	SER	-	expression tag	UNP Q8ST28
D	-16	SER	-	expression tag	UNP Q8ST28
D	-15	HIS	-	expression tag	UNP Q8ST28
D	-14	HIS	-	expression tag	UNP Q8ST28
D	-13	HIS	-	expression tag	UNP Q8ST28
D	-12	HIS	-	expression tag	UNP Q8ST28
D	-11	HIS	-	expression tag	UNP Q8ST28
D	-10	HIS	-	expression tag	UNP Q8ST28
D	-9	SER	-	expression tag	UNP Q8ST28
D	-8	SER	-	expression tag	UNP Q8ST28
D	-7	GLY	-	expression tag	UNP Q8ST28
D	-6	LEU	-	expression tag	UNP Q8ST28
D	-5	VAL	-	expression tag	UNP Q8ST28
D	-4	PRO	-	expression tag	UNP Q8ST28
D	-3	ARG	-	expression tag	UNP Q8ST28
D	-2	GLY	-	expression tag	UNP Q8ST28
D	-1	SER	-	expression tag	UNP Q8ST28
D	0	HIS	-	expression tag	UNP Q8ST28

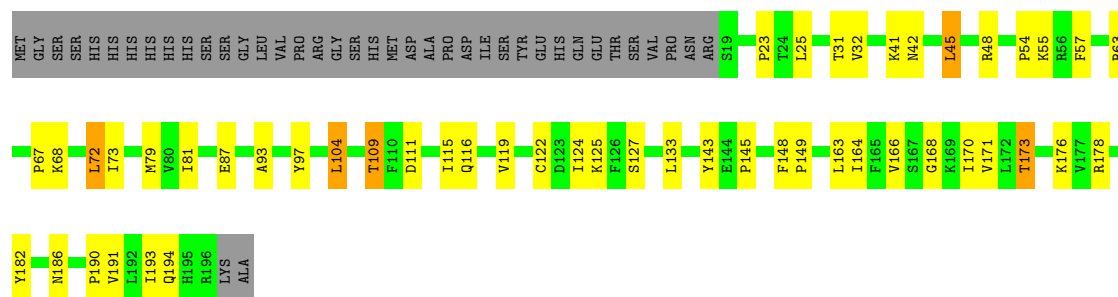
- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	C	1	12	6	1	4	1	0	0
3	D	1	12	6	1	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	11	Total	O	0	0
			11	11		
4	C	4	Total	O	0	0
			4	4		
4	D	2	Total	O	0	0
			2	2		



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.26Å 147.82Å 103.44Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	47.28 – 3.10 47.28 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.28-3.10) 99.9 (47.28-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.187 , 0.242 0.183 , 0.240	Depositor DCC
R_{free} test set	2700 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.020 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15037	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/6203	0.78	9/8365 (0.1%)
1	B	0.37	0/6181	0.78	6/8335 (0.1%)
2	C	0.36	0/1447	0.76	0/1952
2	D	0.39	0/1447	0.76	0/1952
All	All	0.36	0/15278	0.77	15/20604 (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	B	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASP	N-CA-C	8.77	119.50	108.45
1	B	41	ILE	N-CA-C	8.71	120.82	109.58
1	A	41	ILE	N-CA-C	8.03	121.20	109.63
1	B	25	ASP	N-CA-C	7.93	120.50	107.73
1	A	366	VAL	CA-C-N	7.90	127.82	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	TYR	Peptide

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	6086	0	6157	284	0
1	B	6064	0	6130	292	0
2	C	1417	0	1491	48	0
2	D	1417	0	1491	29	0
3	C	12	0	12	1	0
3	D	12	0	12	2	0
4	A	12	0	0	1	0
4	B	11	0	0	0	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
All	All	15037	0	15293	641	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 22.

The worst 5 of 641 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:79:ILE:HD11	1:B:237:ILE:HD11	1.21	1.14
2:D:42:ASN:HD21	3:D:199:MES:H72	1.17	1.09
1:B:19:LEU:HA	1:B:31:ILE:HD11	1.35	1.09
1:A:33:GLU:HG2	1:A:62:ARG:HH22	1.22	1.02
1:A:149:ASN:H	1:A:149:ASN:HD22	1.09	1.00

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	746/800 (93%)	659 (88%)	76 (10%)	11 (2%)	8	32
1	B	743/800 (93%)	655 (88%)	78 (10%)	10 (1%)	9	35
2	C	177/218 (81%)	164 (93%)	12 (7%)	1 (1%)	21	52
2	D	177/218 (81%)	167 (94%)	9 (5%)	1 (1%)	21	52
All	All	1843/2036 (90%)	1645 (89%)	175 (10%)	23 (1%)	10	37

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ILE
1	A	629	ASN
1	B	70	GLN
1	B	487	THR
1	A	24	THR

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	690/727 (95%)	603 (87%)	87 (13%)	4	19
1	B	687/727 (94%)	590 (86%)	97 (14%)	3	15
2	C	154/188 (82%)	133 (86%)	21 (14%)	3	16
2	D	154/188 (82%)	139 (90%)	15 (10%)	8	30
All	All	1685/1830 (92%)	1465 (87%)	220 (13%)	4	17

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	ILE
1	B	424	MET
2	D	186	ASN
2	C	160	ILE

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Mol	Chain	Res	Type
1	B	206	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	95	GLN
2	D	42	ASN
2	C	107	ASN
2	C	186	ASN
1	A	656	HIS

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](#)

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
3	MES	D	199	-	12,12,12	2.29	1 (8%)	15,16,16	2.49	7 (46%)
3	MES	C	199	-	12,12,12	2.31	1 (8%)	15,16,16	2.49	6 (40%)

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
3	MES	D	199	-	-	1/6/14/14	0/1/1/1
3	MES	C	199	-	-	4/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	199	MES	C8-S	-7.70	1.66	1.77
3	D	199	MES	C8-S	-7.65	1.66	1.77

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	199	MES	C5-N4-C3	4.93	119.46	108.84
3	D	199	MES	C5-N4-C3	4.81	119.21	108.84
3	C	199	MES	C6-C5-N4	-3.89	104.21	110.12
3	D	199	MES	C6-C5-N4	-3.75	104.42	110.12
3	D	199	MES	C2-C3-N4	-3.69	104.52	110.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	199	MES	C8-C7-N4-C3
3	C	199	MES	C7-C8-S-O1S
3	C	199	MES	C7-C8-S-O3S
3	D	199	MES	C8-C7-N4-C5
3	C	199	MES	C7-C8-S-O2S

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	199	MES	2	0
3	C	199	MES	1	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	752/800 (94%)	-0.32	3 (0%) 88 76	38, 80, 142, 206	36 (4%)
1	B	749/800 (93%)	-0.43	7 (0%) 81 63	26, 71, 135, 208	23 (3%)
2	C	178/218 (81%)	-0.56	0 100 100	25, 67, 108, 160	3 (1%)
2	D	178/218 (81%)	-0.63	0 100 100	31, 58, 91, 123	4 (2%)
All	All	1857/2036 (91%)	-0.42	10 (0%) 87 73	25, 72, 135, 208	66 (3%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	PHE	3.1
1	B	11	LEU	2.8
1	B	326	LEU	2.6
1	B	146	PRO	2.5
1	B	22	TYR	2.5

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(\AA^2)	Q<0.9
3	MES	C	199	12/12	0.87	0.16	89,103,123,129	0
3	MES	D	199	12/12	0.91	0.10	96,115,130,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.