



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:21 AM UTC

PDB ID : 7QOR / pdb_00007qor
Title : Structure of beta-lactamase TEM-171
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Deposited on : 2021-12-28
Resolution : 2.00 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

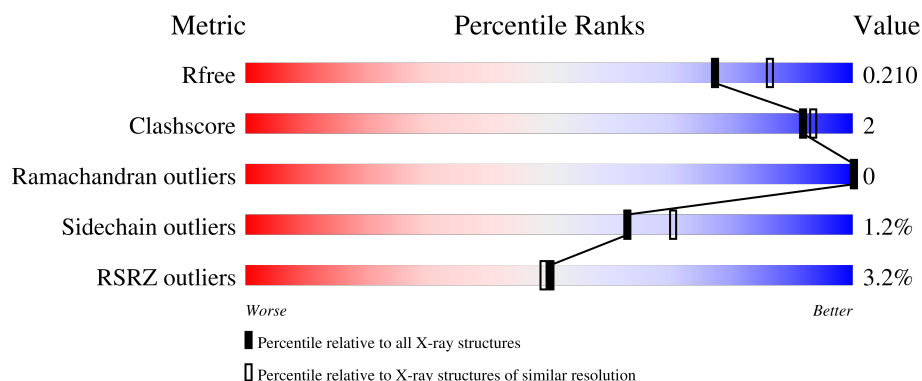
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



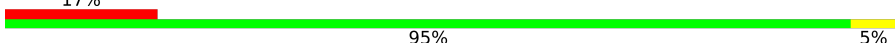
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 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	AAA	263	95% .
1	BBB	263	% 96% .
1	CCC	263	95% 5%
1	DDD	263	95% 5%
1	EEE	263	95% 5%

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Mol	Chain	Length	Quality of chain
1	FFF	263	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	DDD	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13109 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 Beta-lactamase TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	263	Total	C	N	O	S	0	1	0
			2034	1270	360	393	11			
1	BBB	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	CCC	263	Total	C	N	O	S	0	2	0
			2039	1275	362	391	11			
1	DDD	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	EEE	263	Total	C	N	O	S	0	2	0
			2045	1276	365	393	11			
1	FFF	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			

There are 6 discrepancies between the modelled and reference sequences:

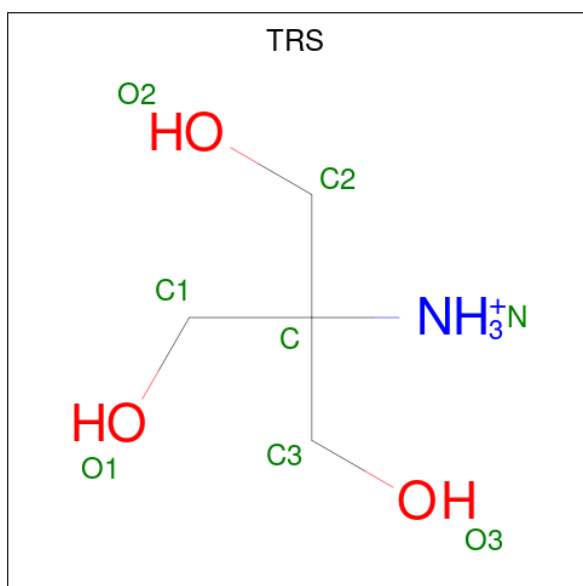
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	84	ILE	VAL	engineered mutation	UNP P62593
BBB	84	ILE	VAL	engineered mutation	UNP P62593
CCC	84	ILE	VAL	engineered mutation	UNP P62593
DDD	84	ILE	VAL	engineered mutation	UNP P62593
EEE	84	ILE	VAL	engineered mutation	UNP P62593
FFF	84	ILE	VAL	engineered mutation	UNP P62593

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



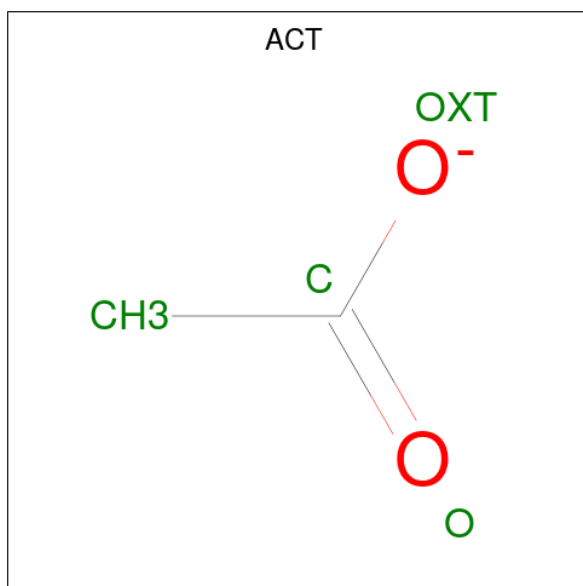
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		
2	CCC	1	Total	C	O	0	0
			4	2	2		
2	CCC	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	CCC	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		
4	DDD	1	Total	C	O	0	0
			4	2	2		

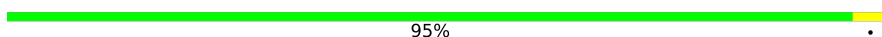
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	238	Total	O	0	0
			238	238		
5	BBB	47	Total	O	0	0
			47	47		
5	CCC	231	Total	O	0	0
			231	231		
5	DDD	155	Total	O	0	0
			155	155		
5	EEE	187	Total	O	0	0
			187	187		
5	FFF	17	Total	O	0	0
			17	17		

3 Residue-property plots [i](#)

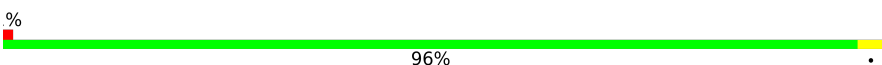
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-lactamase TEM

Chain AAA:  95%

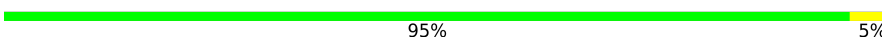


- Molecule 1: Beta-lactamase TEM

Chain BBB:  96%

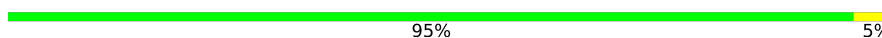


- Molecule 1: Beta-lactamase TEM

Chain CCC:  95%

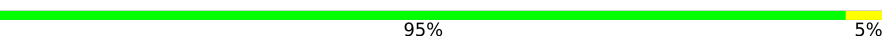


- Molecule 1: Beta-lactamase TEM

Chain DDD:  95%



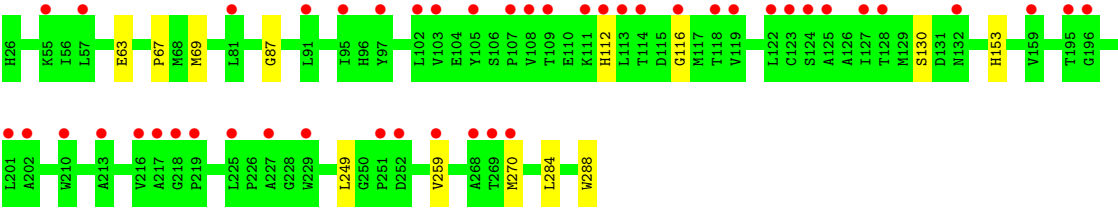
- Molecule 1: Beta-lactamase TEM

Chain EEE:  95%



- Molecule 1: Beta-lactamase TEM

Chain FFF:  17% 95%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.19Å 88.19Å 499.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 15.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.00) 97.8 (15.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.190 , 0.211 0.201 , 0.210	Depositor DCC
R_{free} test set	6653 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13109	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.09% 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: TRS, EDO, ACT

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	AAA	1.04	0/2071	1.31	0/2803
1	BBB	1.04	0/2062	1.40	2/2791 (0.1%)
1	CCC	1.08	1/2080 (0.0%)	1.29	1/2816 (0.0%)
1	DDD	1.07	1/2062 (0.0%)	1.31	0/2791
1	EEE	1.05	0/2082	1.32	0/2817
1	FFF	1.06	0/2062	1.46	0/2791
All	All	1.06	2/12419 (0.0%)	1.35	3/16809 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	220	LEU	N-CA	5.87	1.49	1.46
1	CCC	220	LEU	N-CA	5.63	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	217	ALA	CA-C-N	7.44	126.56	121.13
1	BBB	217	ALA	C-N-CA	7.44	126.56	121.13
1	CCC	204	ARG	CB-CA-C	-5.11	102.64	110.81

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	AAA	2034	0	2042	7	0
1	BBB	2028	0	2036	4	0
1	CCC	2039	0	2052	7	0
1	DDD	2028	0	2036	10	0
1	EEE	2045	0	2056	6	0
1	FFF	2028	0	2036	5	0
2	AAA	4	0	6	0	0
2	CCC	8	0	12	1	0
3	AAA	8	0	12	0	0
4	CCC	4	0	3	0	0
4	DDD	8	0	6	5	0
5	AAA	238	0	0	2	0
5	BBB	47	0	0	0	0
5	CCC	231	0	0	2	0
5	DDD	155	0	0	1	0
5	EEE	187	0	0	0	0
5	FFF	17	0	0	0	0
All	All	13109	0	12297	38	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 2.

The worst 5 of 38 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:AAA:196:GLY:HA3	5:AAA:538:HOH:O	1.72	0.88
1:DDD:43:ARG:HB2	4:DDD:401:ACT:H2	1.75	0.67
1:AAA:70:SER:OG	5:AAA:501:HOH:O	2.13	0.66
1:CCC:70:SER:OG	5:CCC:501:HOH:O	2.10	0.64
1:DDD:43:ARG:HD2	4:DDD:401:ACT:CH3	2.28	0.64

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	AAA	262/263 (100%)	257 (98%)	5 (2%)	0	100	100
1	BBB	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
1	CCC	263/263 (100%)	257 (98%)	6 (2%)	0	100	100
1	DDD	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
1	EEE	263/263 (100%)	257 (98%)	6 (2%)	0	100	100
1	FFF	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
All	All	1571/1578 (100%)	1535 (98%)	36 (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	AAA	218/217 (100%)	215 (99%)	3 (1%)	59	66
1	BBB	217/217 (100%)	214 (99%)	3 (1%)	59	66
1	CCC	219/217 (101%)	218 (100%)	1 (0%)	81	87
1	DDD	217/217 (100%)	215 (99%)	2 (1%)	70	78
1	EEE	219/217 (101%)	217 (99%)	2 (1%)	70	78
1	FFF	217/217 (100%)	213 (98%)	4 (2%)	51	58
All	All	1307/1302 (100%)	1292 (99%)	15 (1%)	63	73

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	63	GLU
1	FFF	153	HIS
1	DDD	153	HIS
1	FFF	270	MET
1	FFF	63	GLU

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
4	ACT	CCC	403	-	3,3,3	1.10	0	3,3,3	0.76	0
4	ACT	DDD	402	-	3,3,3	1.15	0	3,3,3	0.71	0
4	ACT	DDD	401	-	3,3,3	1.12	0	3,3,3	0.42	0
2	EDO	CCC	401	-	3,3,3	0.24	0	2,2,2	0.34	0
2	EDO	CCC	402	-	3,3,3	0.43	0	2,2,2	0.39	0
3	TRS	AAA	402	-	7,7,7	0.32	0	9,9,9	0.54	0
2	EDO	AAA	401	-	3,3,3	0.66	0	2,2,2	0.83	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
3	TRS	AAA	402	-	-	0/9/9/9	-
2	EDO	AAA	401	-	-	1/1/1/1	-
2	EDO	CCC	401	-	-	1/1/1/1	-
2	EDO	CCC	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CCC	401	EDO	O1-C1-C2-O2
2	AAA	401	EDO	O1-C1-C2-O2
2	CCC	402	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	401	ACT	5	0
2	CCC	401	EDO	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	AAA	263/263 (100%)	-0.37	0 100 100	32, 43, 59, 70	1 (0%)
1	BBB	263/263 (100%)	0.44	3 (1%) 78 77	62, 77, 99, 111	0
1	CCC	263/263 (100%)	-0.39	1 (0%) 88 88	22, 40, 55, 66	2 (0%)
1	DDD	263/263 (100%)	-0.25	0 100 100	36, 48, 66, 78	0
1	EEE	263/263 (100%)	-0.19	0 100 100	22, 51, 72, 81	2 (0%)
1	FFF	263/263 (100%)	1.21	46 (17%) 4 3	70, 105, 150, 170	0
All	All	1578/1578 (100%)	0.07	50 (3%) 50 49	22, 53, 124, 170	5 (0%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FFF	103	VAL	4.5
1	FFF	108	VAL	4.0
1	FFF	201	LEU	4.0
1	FFF	128	THR	3.7
1	FFF	118	THR	3.4

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(Å ²)	Q<0.9
4	ACT	DDD	402	4/4	0.47	0.16	79,80,82,85	0
3	TRS	AAA	402	8/8	0.61	0.14	56,76,78,81	0
4	ACT	CCC	403	4/4	0.64	0.14	78,84,85,87	0
2	EDO	CCC	401	4/4	0.89	0.11	72,72,73,73	0
2	EDO	AAA	401	4/4	0.93	0.09	49,49,51,51	0
4	ACT	DDD	401	4/4	0.94	0.08	60,60,61,62	0
2	EDO	CCC	402	4/4	0.96	0.07	49,51,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.