



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:56 pm BST

PDB ID : 1XWL
Title : BACILLUS STEAROTHERMOPHILUS (NEWLY IDENTIFIED STRAIN AS YET UNNAMED) DNA POLYMERASE FRAGMENT
Authors : Kiefer, J.R.; Mao, C.; Beese, L.S.
Deposited on : 1998-07-22
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

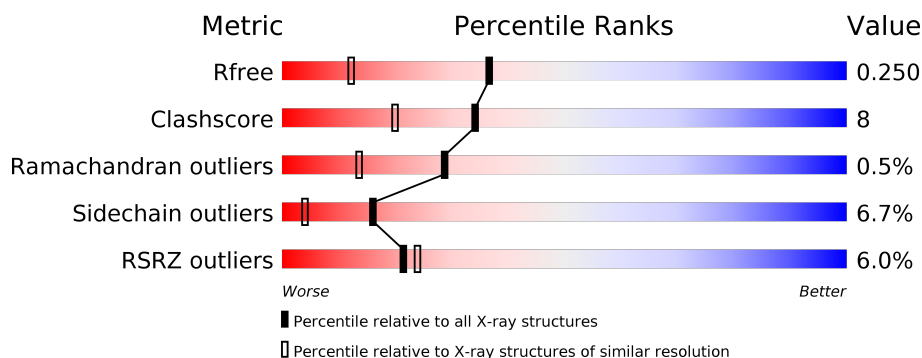
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	580	<div> <div>6%</div> <div>78%</div> <div>19%</div> </div>

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
2	SO4	A	901	-	X	-	-
2	SO4	A	902	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5069 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 DNA POLYMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	580	4654	2959	808	870	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	GLU	ALA	SEE REMARK 999	UNP P52026
A	505	LYS	GLU	SEE REMARK 999	UNP P52026
A	512	GLY	ARG	SEE REMARK 999	UNP P52026
A	550	THR	SER	SEE REMARK 999	UNP P52026
A	?	-	GLN	DELETION	UNP P52026
A	823	HIS	ARG	SEE REMARK 999	UNP P52026

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

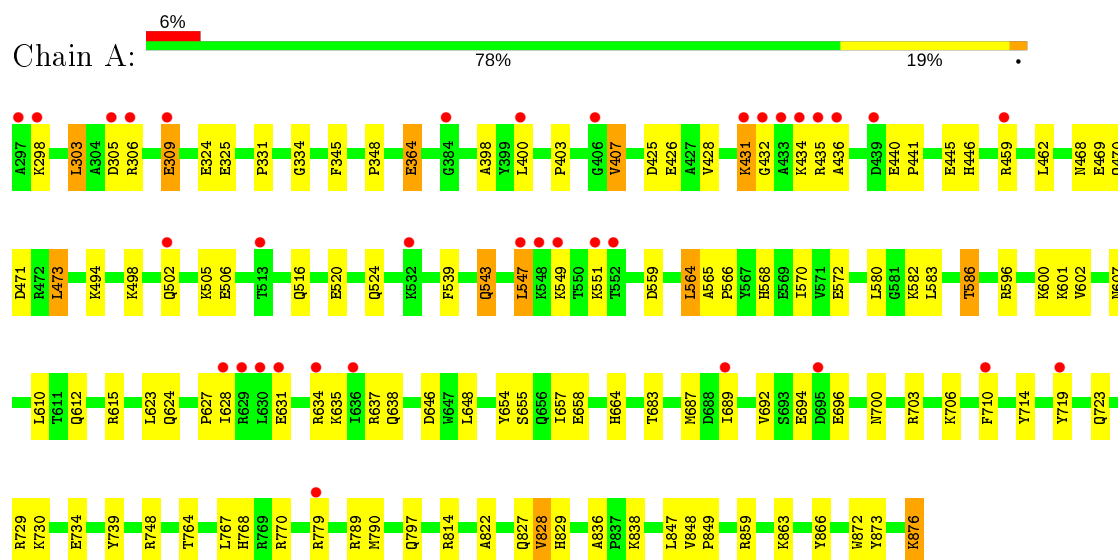
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	405	Total	O	0	0
			405	405		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 POLYMERASE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.11Å 93.87Å 104.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 19.88 – 1.70	Depositor EDS
% Data completeness (in resolution range)	89.3 (20.00-1.70) 94.0 (19.88-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 1.70Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.254 , 0.291 0.207 , 0.250	Depositor DCC
R_{free} test set	4491 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5069	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: SO4

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	0.51	0/4738	0.68	0/6402

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	714	TYR	Sidechain

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	4654	0	4709	79	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	405	0	0	3	0
All	All	5069	0	4709	79	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 8.

All (79) 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:A:700:ASN:HD21	1:A:703:ARG:HH21	1.19	0.87
1:A:624:GLN:HE21	1:A:829:HIS:H	1.24	0.82
1:A:502:GLN:O	1:A:506:GLU:HG3	1.81	0.80
1:A:748:ARG:HG2	1:A:748:ARG:HH11	1.48	0.78
1:A:568:HIS:HD2	1:A:570:ILE:H	1.30	0.77
1:A:426:GLU:CD	1:A:431:LYS:HG3	2.07	0.75
1:A:683:THR:HG22	1:A:687:MET:HE3	1.68	0.74
1:A:646:ASP:HA	1:A:838:LYS:HZ3	1.52	0.73
1:A:543:GLN:HE21	1:A:543:GLN:HA	1.55	0.72
1:A:520:GLU:HA	1:A:520:GLU:OE1	1.89	0.71
1:A:683:THR:HG22	1:A:687:MET:CE	2.21	0.71
1:A:700:ASN:ND2	1:A:703:ARG:HH21	1.89	0.71
1:A:687:MET:HE1	1:A:694:GLU:HB2	1.74	0.70
1:A:635:LYS:HE2	1:A:873:TYR:OH	1.91	0.68
1:A:624:GLN:HA	1:A:828:VAL:HG22	1.77	0.67
1:A:624:GLN:NE2	1:A:829:HIS:H	1.94	0.65
1:A:658:GLU:OE2	1:A:797:GLN:HG2	1.98	0.63
1:A:692:VAL:HB	1:A:696:GLU:HB2	1.82	0.61
1:A:615:ARG:HE	1:A:797:GLN:HE21	1.47	0.60
1:A:303:LEU:HD13	1:A:345:PHE:HD2	1.68	0.59
1:A:730:LYS:HE2	1:A:734:GLU:OE2	2.05	0.57
1:A:822:ALA:CB	1:A:836:ALA:HB2	2.34	0.56
1:A:624:GLN:HE21	1:A:829:HIS:N	1.99	0.56
1:A:873:TYR:O	1:A:876:LYS:HD2	2.06	0.56
1:A:468:ASN:HD22	1:A:470:GLN:NE2	2.04	0.55
1:A:434:LYS:O	1:A:436:ALA:N	2.40	0.55
1:A:687:MET:CE	1:A:694:GLU:HB2	2.37	0.55
1:A:637:ARG:HG2	1:A:872:TRP:CD2	2.42	0.54
1:A:539:PHE:CE1	1:A:564:LEU:HD11	2.43	0.54
1:A:848:VAL:HB	1:A:849:PRO:HD3	1.89	0.53
1:A:646:ASP:HA	1:A:838:LYS:NZ	2.22	0.53
1:A:572:GLU:HB3	3:A:1348:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:LYS:HD3	1:A:873:TYR:CE1	2.45	0.51
1:A:309:GLU:HG3	1:A:309:GLU:O	2.10	0.51
1:A:494:LYS:HE3	1:A:600:LYS:HB2	1.94	0.50
1:A:748:ARG:HG2	1:A:748:ARG:NH1	2.24	0.49
1:A:687:MET:HE2	1:A:694:GLU:HA	1.94	0.49
1:A:400:LEU:HD22	1:A:473:LEU:HD13	1.95	0.49
1:A:767:LEU:O	1:A:768:HIS:HB2	2.13	0.48
1:A:440:GLU:N	1:A:441:PRO:HD2	2.29	0.47
1:A:547:LEU:HD22	3:A:1347:HOH:O	2.14	0.47
1:A:565:ALA:HB3	1:A:566:PRO:HD3	1.95	0.47
1:A:634:ARG:HH22	1:A:876:LYS:HG3	1.80	0.47
1:A:719:TYR:CZ	1:A:729:ARG:HD3	2.50	0.47
1:A:624:GLN:HA	1:A:828:VAL:CG2	2.44	0.46
1:A:689:ILE:HD11	1:A:739:TYR:HB2	1.96	0.46
1:A:789:ARG:NH1	1:A:790:MET:HE1	2.30	0.46
1:A:364:GLU:O	1:A:364:GLU:HG3	2.14	0.46
1:A:664:HIS:O	1:A:859:ARG:NH1	2.48	0.46
1:A:568:HIS:CD2	1:A:570:ILE:H	2.21	0.46
1:A:654:TYR:HB3	1:A:657:ILE:HB	1.98	0.45
1:A:334:GLY:HA2	1:A:348:PRO:HD3	1.98	0.45
1:A:624:GLN:CA	1:A:828:VAL:HG22	2.44	0.45
1:A:425:ASP:OD1	1:A:446:HIS:HE1	2.00	0.44
1:A:635:LYS:HE2	1:A:873:TYR:CZ	2.52	0.44
1:A:637:ARG:HG2	1:A:872:TRP:CE3	2.52	0.44
1:A:764:THR:HG22	1:A:770:ARG:HG2	1.99	0.44
1:A:582:LYS:O	1:A:586:THR:CG2	2.66	0.43
1:A:849:PRO:HG3	1:A:866:TYR:CD1	2.54	0.43
1:A:583:LEU:HD13	1:A:627:PRO:HG2	1.99	0.43
1:A:648:LEU:HG	1:A:838:LYS:HG2	2.01	0.43
1:A:403:PRO:HB2	1:A:612:GLN:HG2	2.01	0.43
1:A:582:LYS:O	1:A:586:THR:HG23	2.19	0.43
1:A:624:GLN:HG3	1:A:828:VAL:HG22	2.00	0.43
1:A:398:ALA:HB1	1:A:407:VAL:HG21	2.01	0.42
1:A:814:ARG:CZ	1:A:847:LEU:HD11	2.49	0.42
1:A:635:LYS:HE2	1:A:873:TYR:HH	1.82	0.42
1:A:428:VAL:HG21	1:A:446:HIS:CD2	2.54	0.42
1:A:324:GLU:HG3	1:A:331:PRO:HD2	2.01	0.42
1:A:628:ILE:HG13	1:A:628:ILE:H	1.71	0.41
1:A:303:LEU:HD13	1:A:345:PHE:CD2	2.52	0.41
1:A:655:SER:OG	1:A:863:LYS:HG2	2.19	0.41
1:A:607:ASN:HB2	3:A:1270:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASP:N	1:A:471:ASP:OD1	2.49	0.41
1:A:596:ARG:HG2	1:A:601:LYS:O	2.21	0.41
1:A:648:LEU:HD11	1:A:838:LYS:HD3	2.03	0.41
1:A:706:LYS:O	1:A:710:PHE:HD1	2.03	0.41
1:A:635:LYS:HD2	1:A:638:GLN:NE2	2.36	0.40
1:A:462:LEU:HA	1:A:462:LEU:HD23	1.95	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
1	A	578/580 (100%)	561 (97%)	14 (2%)	3 (0%)	29 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	407	VAL
1	A	435	ARG
1	A	432	GLY

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	496/496 (100%)	463 (93%)	33 (7%)	16 4

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	LYS
1	A	303	LEU
1	A	305	ASP
1	A	306	ARG
1	A	309	GLU
1	A	325	GLU
1	A	364	GLU
1	A	431	LYS
1	A	445	GLU
1	A	459	ARG
1	A	469	GLU
1	A	473	LEU
1	A	498	LYS
1	A	505	LYS
1	A	516	GLN
1	A	524	GLN
1	A	543	GLN
1	A	547	LEU
1	A	549	LYS
1	A	551	LYS
1	A	559	ASP
1	A	564	LEU
1	A	580	LEU
1	A	586	THR
1	A	602	VAL
1	A	610	LEU
1	A	623	LEU
1	A	631	GLU
1	A	723	GLN
1	A	779	ARG
1	A	827	GLN
1	A	828	VAL
1	A	876	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	446	HIS
1	A	470	GLN
1	A	543	GLN
1	A	568	HIS
1	A	573	ASN
1	A	624	GLN
1	A	691	GLN
1	A	700	ASN
1	A	709	ASN
1	A	797	GLN
1	A	812	ASN
1	A	827	GLN
1	A	829	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 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	SO4	A	901	-	4,4,4	2.41	4 (100%)	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	902	-	4,4,4	2.48	4 (100%)	6,6,6	0.23	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	SO4	O4-S	2.61	1.69	1.47
2	A	902	SO4	O3-S	2.59	1.69	1.47
2	A	902	SO4	O4-S	2.55	1.68	1.47
2	A	902	SO4	O1-S	2.50	1.59	1.46
2	A	901	SO4	O3-S	2.49	1.68	1.47
2	A	902	SO4	O2-S	2.28	1.58	1.46
2	A	901	SO4	O2-S	2.26	1.58	1.46
2	A	901	SO4	O1-S	2.24	1.58	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	580/580 (100%)	0.21	35 (6%)	21 24	11, 20, 40, 62	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ALA	8.1
1	A	433	ALA	7.8
1	A	432	GLY	6.8
1	A	551	LYS	6.5
1	A	431	LYS	5.5
1	A	629	ARG	5.3
1	A	298	LYS	4.4
1	A	434	LYS	4.3
1	A	628	ILE	4.1
1	A	549	LYS	4.0
1	A	406	GLY	3.9
1	A	547	LEU	3.7
1	A	630	LEU	3.6
1	A	552	THR	3.5
1	A	306	ARG	3.5
1	A	309	GLU	2.9
1	A	634	ARG	2.8
1	A	719	TYR	2.8
1	A	459	ARG	2.8
1	A	779	ARG	2.8
1	A	548	LYS	2.6
1	A	513	THR	2.5
1	A	689	ILE	2.5
1	A	695	ASP	2.4
1	A	636	ILE	2.3
1	A	710	PHE	2.2
1	A	436	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	502	GLN	2.1
1	A	631	GLU	2.1
1	A	439	ASP	2.1
1	A	435	ARG	2.0
1	A	305	ASP	2.0
1	A	384	GLY	2.0
1	A	532	LYS	2.0
1	A	400	LEU	2.0

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. 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
2	SO4	A	901	5/5	0.94	0.12	40,41,42,43	0
2	SO4	A	902	5/5	0.94	0.17	45,45,47,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.