



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:11 am BST

PDB ID : 2ONL
Title : Crystal Structure of the p38a-MAPKAP kinase 2 Heterodimer
Authors : Ter Haar, E.
Deposited on : 2007-01-24
Resolution : 4.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

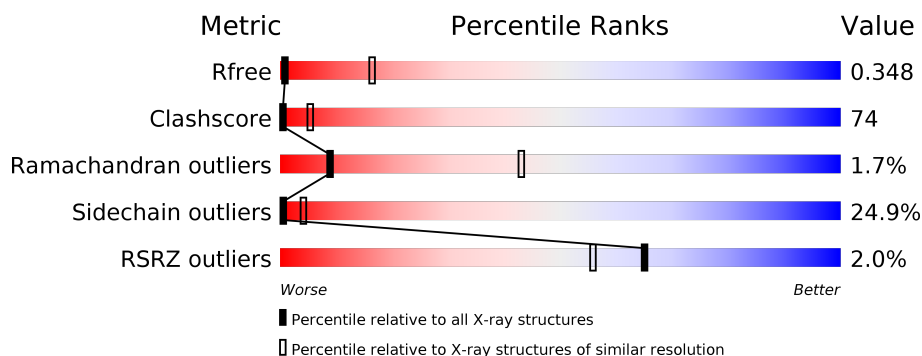
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	366	<div> <div>2%</div> <div>36% 45% 11% 8%</div> </div>
1	B	366	<div> <div>%</div> <div>33% 48% 11% 7%</div> </div>
2	C	406	<div> <div>2%</div> <div>10% 43% 23% 22%</div> </div>
2	D	406	<div> <div>%</div> <div>14% 42% 19% 23%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10466 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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2709	1737	466	494	12			
1	B	339	Total	C	N	O	S	0	0	0
			2714	1740	467	495	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP Q16539
A	-4	SER	-	CLONING ARTIFACT	UNP Q16539
A	-3	HIS	-	CLONING ARTIFACT	UNP Q16539
A	-2	MET	-	CLONING ARTIFACT	UNP Q16539
A	-1	LEU	-	CLONING ARTIFACT	UNP Q16539
A	0	GLU	-	CLONING ARTIFACT	UNP Q16539
A	1	MET	-	CLONING ARTIFACT	UNP Q16539
B	-5	GLY	-	CLONING ARTIFACT	UNP Q16539
B	-4	SER	-	CLONING ARTIFACT	UNP Q16539
B	-3	HIS	-	CLONING ARTIFACT	UNP Q16539
B	-2	MET	-	CLONING ARTIFACT	UNP Q16539
B	-1	LEU	-	CLONING ARTIFACT	UNP Q16539
B	0	GLU	-	CLONING ARTIFACT	UNP Q16539
B	1	MET	-	CLONING ARTIFACT	UNP Q16539

- Molecule 2 is a protein called MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	317	Total	C	N	O	S	0	0	0
			2531	1611	440	462	18			
2	D	313	Total	C	N	O	S	0	0	0
			2512	1597	437	460	18			

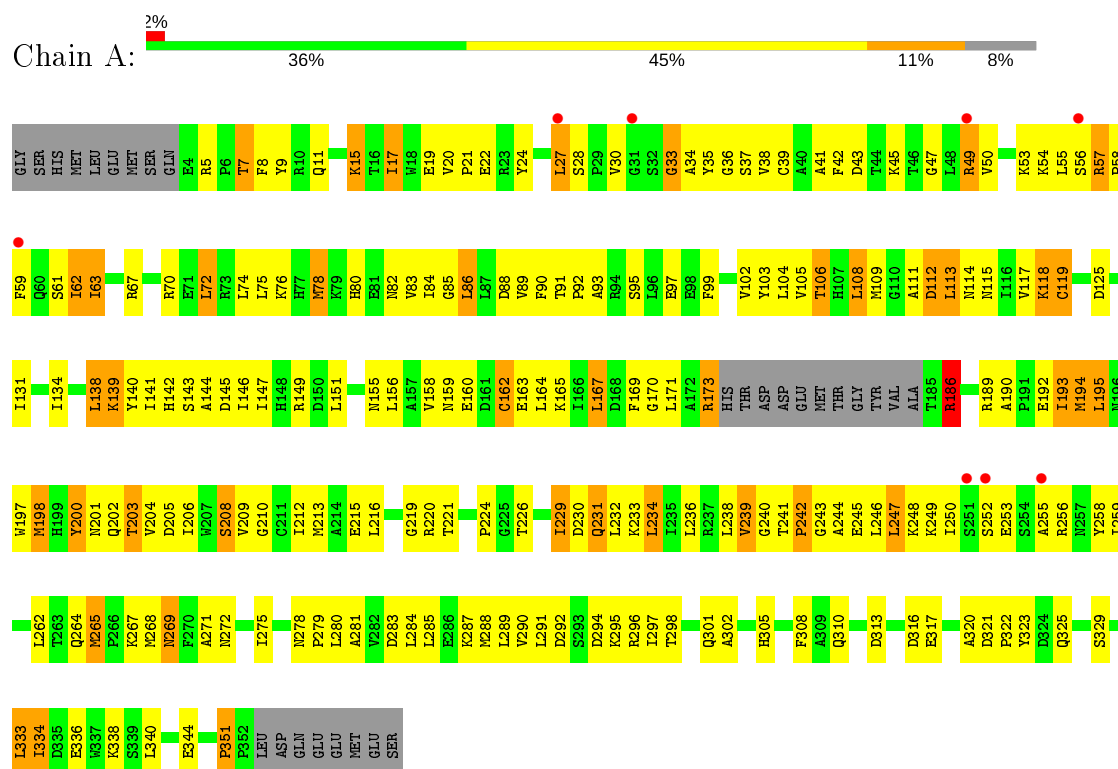
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	CLONING ARTIFACT	UNP P49137
C	-4	SER	-	CLONING ARTIFACT	UNP P49137
C	-3	HIS	-	CLONING ARTIFACT	UNP P49137
C	-2	MET	-	CLONING ARTIFACT	UNP P49137
C	-1	LEU	-	CLONING ARTIFACT	UNP P49137
C	0	GLU	-	CLONING ARTIFACT	UNP P49137
D	-5	GLY	-	CLONING ARTIFACT	UNP P49137
D	-4	SER	-	CLONING ARTIFACT	UNP P49137
D	-3	HIS	-	CLONING ARTIFACT	UNP P49137
D	-2	MET	-	CLONING ARTIFACT	UNP P49137
D	-1	LEU	-	CLONING ARTIFACT	UNP P49137
D	0	GLU	-	CLONING ARTIFACT	UNP P49137

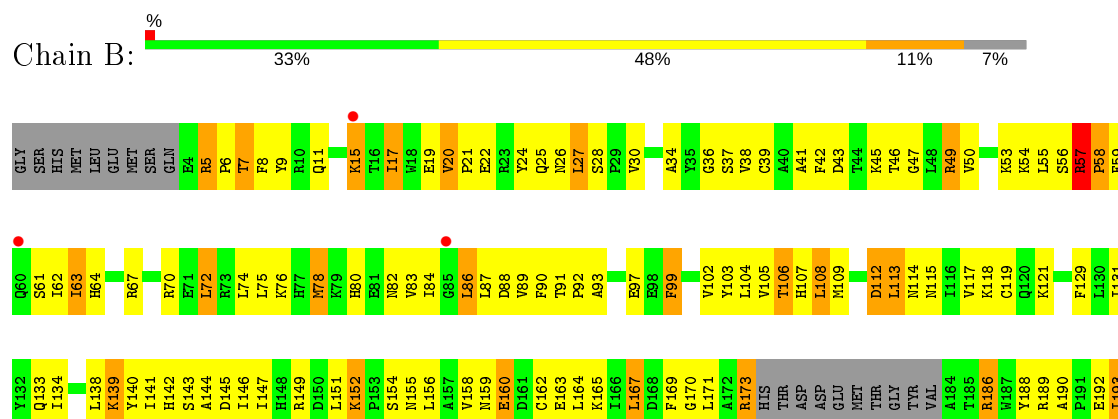
3 Residue-property plots

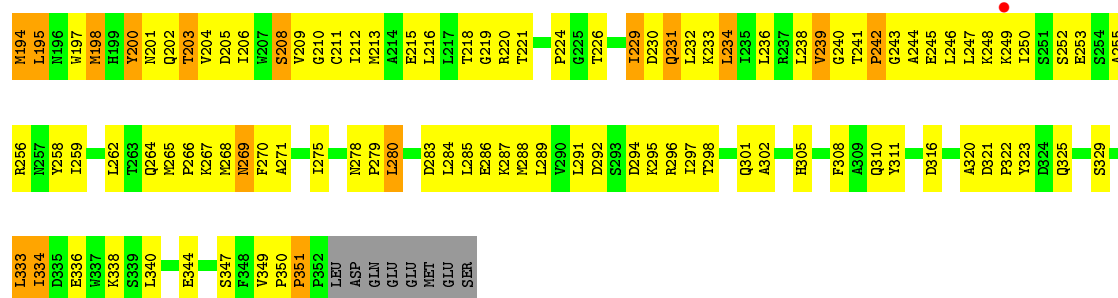
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Mitogen-activated protein kinase 14



- Molecule 1: Mitogen-activated protein kinase 14





A359	L360	A361	T362	M363	R364	V365	D366	Q369	T370	K371	I372	K373	D377	A378	S379	N380	P381	L382	L383	L384	K385	R386	R387	K388	K389	L393	GLU	ALA	ALA	ALA	LEU	ALA	HIS																										
V298	K299	N300	L301	I302	R303	N304	L305	L306	K307	T308	E309	P310	T311	Q312	R313	R314	T315	I316	T317	E318	F319	K320	N321	R322	P323	K324	I325	K326	D327	S328	T329	K330	V331	T334	P335	L336	R337	T338	S339	R340	V341	L342	K343	D344	D345	K346	E347	R348	K349	E350	D351	V352	K353	E354	E355	K356	T357	S358	
E238	K239	Y240	D241	K242	S243	C244	D245	N246	W247	S248	L249	G250	V251	I252	M253	Y254	I255	L256	L257	C258	G259	Y260	P261	P262	P263	TYR	SER	ASN	HIS	GLY	LEU	ALA	ILE	SER	PRO	GLY	MET	LYS	THR	ARG	ILE	ARG	MET	GLY	GLN	Y284	E285	F286	P287	N288	P289	E290	W291	S292	E293	V294	S295	E296	E297
H178	S179	I180	N181	I182	A183	H184	A185	D186	V187	K188	P189	E190	N191	L192	L193	Y194	T195	S196	K197	R198	P199	N200	A201	I202	L203	L204	L205	T206	D207	F208	G209	F210	A211	K212	E213	T214	T215	S216	E217	K218	S219	L220	T221	T222	P223	C224	Y225	T226	P227	Y228	Y229	V230	A231	P232	E233	V234	L235	G236	P237

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	103.15Å 103.15Å 231.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.34 – 4.00 45.34 – 4.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (45.34-4.00) 95.9 (45.34-4.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 4.00Å)	Xtriage
Refinement program	BUSTER-TNT V. 1.1.0	Depositor
R, R_{free}	0.314 , 0.331 0.340 , 0.348	Depositor DCC
R_{free} test set	984 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	106.4	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.219 for h,-k,-l	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	10466	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

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	0.27	0/2770	0.51	2/3758 (0.1%)
1	B	0.26	0/2775	0.48	2/3765 (0.1%)
2	C	0.25	0/2583	0.59	3/3480 (0.1%)
2	D	0.32	2/2563 (0.1%)	0.57	4/3453 (0.1%)
All	All	0.28	2/10691 (0.0%)	0.54	11/14456 (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	2
1	B	0	1
2	C	0	24
2	D	0	25
All	All	0	52

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	354	GLU	CD-OE2	6.41	1.32	1.25
2	D	354	GLU	CD-OE1	5.65	1.31	1.25

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	231	ALA	C-N-CD	-7.96	103.09	120.60
2	C	194	TYR	CB-CA-C	-7.67	95.06	110.40
1	A	265	MET	N-CA-C	7.67	131.71	111.00
2	C	234	VAL	N-CA-C	6.29	128.00	111.00
2	D	237	PRO	N-CA-CB	5.93	110.41	103.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Peptide
1	A	33	GLY	Peptide
2	C	153	ARG	Peptide
2	C	154	GLY	Peptide
2	C	89	LYS	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	2709	0	2701	298	0
1	B	2714	0	2706	325	0
2	C	2531	0	2509	517	6
2	D	2512	0	2500	495	2
All	All	10466	0	10416	1540	8

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 74.

The worst 5 of 1540 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:159:ASN:C	2:D:370:ILE:HD13	1.35	1.42
2:D:214:THR:HG23	2:D:237:PRO:O	1.24	1.37
2:C:315:THR:CG2	2:C:318:GLU:CB	2.02	1.36
2:D:214:THR:CG2	2:D:238:GLU:HA	1.58	1.33
2:D:99:PRO:O	2:D:103:ARG:HG3	1.22	1.32

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:ALA:CB	2:C:226:THR:OG1[4_574]	1.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:58:ALA:CA	2:C:226:THR:OG1[4_574]	1.75	0.45
2:D:58:ALA:CA	2:D:226:THR:O[3_745]	1.87	0.33
2:D:58:ALA:N	2:D:226:THR:O[3_745]	1.87	0.33
2:C:58:ALA:N	2:C:226:THR:CG2[4_574]	1.90	0.30

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	334/366 (91%)	307 (92%)	25 (8%)	2 (1%)	25	63
1	B	335/366 (92%)	309 (92%)	23 (7%)	3 (1%)	17	55
2	C	311/406 (77%)	262 (84%)	40 (13%)	9 (3%)	4	32
2	D	307/406 (76%)	247 (80%)	52 (17%)	8 (3%)	5	34
All	All	1287/1544 (83%)	1125 (87%)	140 (11%)	22 (2%)	9	43

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	237	PRO
2	D	232	PRO
2	D	237	PRO
2	C	222	THR
2	C	232	PRO

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	294/325 (90%)	240 (82%)	54 (18%)	1	10
1	B	294/325 (90%)	243 (83%)	51 (17%)	2	13
2	C	272/362 (75%)	182 (67%)	90 (33%)	0	2
2	D	273/362 (75%)	186 (68%)	87 (32%)	0	2
All	All	1133/1374 (82%)	851 (75%)	282 (25%)	0	4

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	351	ASP
1	B	78	MET
2	D	313	ARG
2	C	360	LEU
2	C	389	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	HIS
1	B	202	GLN
2	D	288	ASN
1	B	114	ASN
1	B	228	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	338/366 (92%)	0.08	8 (2%) 59 49	100, 100, 100, 100	0
1	B	339/366 (92%)	-0.04	4 (1%) 79 70	100, 100, 100, 100	0
2	C	317/406 (78%)	0.09	9 (2%) 53 42	20, 100, 100, 100	0
2	D	313/406 (77%)	0.00	5 (1%) 72 62	100, 100, 100, 100	0
All	All	1307/1544 (84%)	0.03	26 (1%) 65 56	20, 100, 100, 100	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	SER	6.0
1	A	252	SER	4.1
1	A	56	SER	3.9
2	C	202	ILE	3.7
1	B	85	GLY	2.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.