Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 07:30 PM EST

PDB ID	:	3QXL
Title	:	Crystal structure of the CDC25 Domain from Ral-specific Guanine-nucleotide Exchange Factor RalGPS1a
Authors	:	Peng, W.; Xu, J.; Guan, X.; Sun, Y.; Li, X.; Zhang, X.C.; Rao, Z.
Deposited on	:	2011-03-02
Resolution	:	2.24 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 (i) 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 (1)) were used in the production of this report:

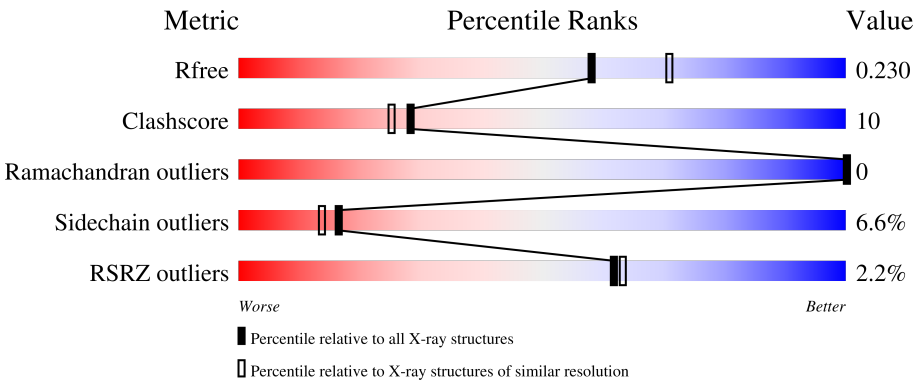
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 <=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	271	3% 75% 12% • 10%
1	B	271	% 70% 17% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4136 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 Ras-specific guanine nucleotide-releasing factor RalGPS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	2010	1298	338	366	8	0	0	0
1	B	244	2002	1294	337	363	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP Q5JS13
A	20	PRO	-	expression tag	UNP Q5JS13
A	21	LEU	-	expression tag	UNP Q5JS13
A	22	GLY	-	expression tag	UNP Q5JS13
B	19	GLY	-	expression tag	UNP Q5JS13
B	20	PRO	-	expression tag	UNP Q5JS13
B	21	LEU	-	expression tag	UNP Q5JS13
B	22	GLY	-	expression tag	UNP Q5JS13

- Molecule 2 is water.

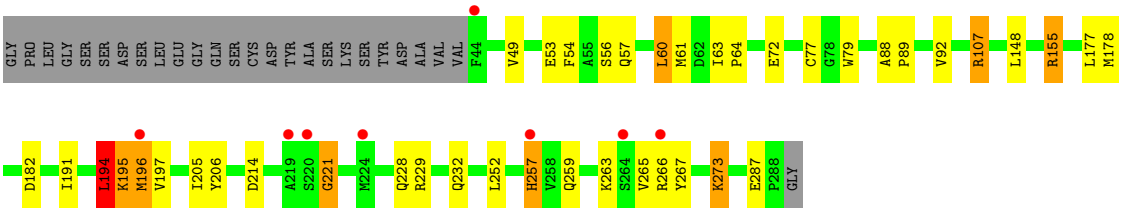
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	68	68	68	0	0
2	B	56	56	56	0	0

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.

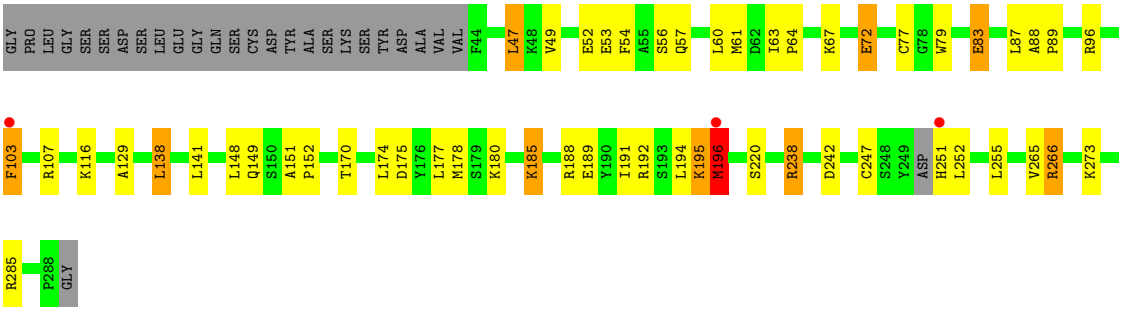
• Molecule 1: Ras-specific guanine nucleotide-releasing factor RalGPS1

Chain A:



• Molecule 1: Ras-specific guanine nucleotide-releasing factor RalGPS1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	36.50Å 102.03Å 82.14Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	40.80 – 2.24 43.26 – 2.24	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.80-2.24) 94.9 (43.26-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.197 , 0.240 0.191 , 0.230	Depositor DCC
R_{free} test set	1394 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4136	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.80	2/2051 (0.1%)	0.75	6/2774 (0.2%)
1	B	0.55	3/2042 (0.1%)	0.56	4/2760 (0.1%)
All	All	0.69	5/4093 (0.1%)	0.66	10/5534 (0.2%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	GLY	CA-C	-29.50	1.04	1.51
1	B	220	SER	C-N	-11.83	1.11	1.33
1	B	72	GLU	CG-CD	8.29	1.64	1.51
1	A	221	GLY	N-CA	-7.79	1.34	1.46
1	B	72	GLU	CB-CG	5.18	1.61	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	GLY	N-CA-C	20.46	164.25	113.10
1	A	221	GLY	CA-C-O	-14.34	94.78	120.60
1	A	221	GLY	CA-C-N	9.28	137.61	117.20
1	A	196	MET	CB-CA-C	-7.93	94.55	110.40
1	B	220	SER	O-C-N	-7.40	110.61	123.20
1	B	220	SER	C-N-CA	6.96	136.92	122.30
1	B	220	SER	CA-C-N	6.03	128.27	116.20
1	A	194	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	196	MET	CB-CA-C	-5.25	99.91	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	VAL	N-CA-CB	5.02	122.55	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	GLY	Mainchain

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	2010	0	2070	32	0
1	B	2002	0	2064	48	0
2	A	68	0	0	1	0
2	B	56	0	0	1	0
All	All	4136	0	4134	80	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 (80) 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:195:LYS:NZ	1:B:195:LYS:HB3	1.73	1.02
1:B:195:LYS:O	1:B:196:MET:HB2	1.62	0.95
1:A:257:HIS:H	1:A:257:HIS:CD2	1.78	0.91
1:A:195:LYS:O	1:A:196:MET:HB2	1.76	0.84
1:B:195:LYS:HB3	1:B:195:LYS:HZ2	1.46	0.81
1:A:259:GLN:O	1:A:263:LYS:HG3	1.79	0.81
1:B:195:LYS:NZ	1:B:195:LYS:CB	2.47	0.77
1:B:195:LYS:HB3	1:B:195:LYS:HZ3	1.52	0.74
1:B:103:PHE:HE1	1:B:107:ARG:HH11	1.30	0.74
1:A:273:LYS:N	1:A:273:LYS:HD2	2.03	0.73
1:B:67:LYS:HE2	1:B:247:CYS:O	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LYS:HZ2	1:B:195:LYS:CB	2.01	0.73
1:A:107:ARG:CG	1:A:107:ARG:HH21	2.06	0.69
1:B:103:PHE:HE1	1:B:107:ARG:NH1	1.92	0.68
1:A:228:GLN:NE2	1:A:232:GLN:HE21	1.92	0.68
1:B:103:PHE:CZ	1:B:107:ARG:HD3	2.29	0.67
1:B:49:VAL:HB	1:B:54:PHE:CE2	2.31	0.66
1:B:77:CYS:HA	1:B:79:TRP:CZ3	2.31	0.66
1:A:214:ASP:OD1	1:A:229:ARG:NH2	2.28	0.65
1:B:56:SER:HB2	1:B:252:LEU:HD22	1.82	0.62
1:B:103:PHE:CE1	1:B:107:ARG:NH1	2.63	0.60
1:A:155:ARG:NH2	1:A:287:GLU:O	2.28	0.60
1:A:257:HIS:CD2	1:A:257:HIS:N	2.59	0.60
1:B:103:PHE:CD2	2:B:293:HOH:O	2.52	0.59
1:A:177:LEU:HG	1:A:178:MET:HE2	1.85	0.58
1:A:77:CYS:HA	1:A:79:TRP:CZ3	2.38	0.58
1:A:56:SER:HB2	1:A:252:LEU:HD22	1.86	0.57
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.87	0.56
1:B:195:LYS:O	1:B:196:MET:CB	2.41	0.56
1:B:185:LYS:HD2	1:B:189:GLU:OE2	2.06	0.55
1:B:67:LYS:CE	1:B:247:CYS:O	2.56	0.53
1:A:195:LYS:O	1:A:196:MET:CB	2.52	0.52
1:B:77:CYS:HA	1:B:79:TRP:CH2	2.45	0.52
1:B:185:LYS:O	1:B:189:GLU:HG3	2.10	0.52
1:B:177:LEU:HG	1:B:178:MET:HE2	1.93	0.51
1:B:57:GLN:O	1:B:61:MET:HG3	2.12	0.50
1:A:107:ARG:HH21	1:A:107:ARG:HG2	1.74	0.50
1:A:107:ARG:CG	1:A:107:ARG:NH2	2.69	0.49
1:A:191:ILE:HA	1:A:194:LEU:HD22	1.95	0.49
1:B:188:ARG:O	1:B:191:ILE:HG22	2.13	0.48
1:A:273:LYS:HD2	1:A:273:LYS:H	1.77	0.48
1:A:177:LEU:HG	1:A:178:MET:CE	2.43	0.48
1:A:266:ARG:HG2	1:A:267:TYR:N	2.28	0.48
1:B:103:PHE:CE1	1:B:107:ARG:HD3	2.49	0.48
1:B:53:GLU:HG2	1:B:255:LEU:HD11	1.96	0.47
1:B:103:PHE:CZ	1:B:265:VAL:HG11	2.49	0.47
1:B:189:GLU:HG2	1:B:192:ARG:HH12	1.79	0.47
1:B:185:LYS:HD2	1:B:189:GLU:CD	2.36	0.46
1:A:265:VAL:HG12	1:A:265:VAL:O	2.15	0.46
1:B:83:GLU:HG2	1:B:87:LEU:HD11	1.99	0.45
1:A:267:TYR:HA	2:A:342:HOH:O	2.17	0.45
1:B:138:LEU:CD2	1:B:191:ILE:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLN:O	1:A:61:MET:HG3	2.17	0.44
1:A:107:ARG:NH2	1:A:107:ARG:HG3	2.33	0.44
1:B:138:LEU:HD22	1:B:191:ILE:HD13	2.00	0.44
1:B:196:MET:N	1:B:196:MET:SD	2.88	0.44
1:B:63:ILE:N	1:B:64:PRO:CD	2.81	0.43
1:A:228:GLN:HE21	1:A:232:GLN:HE21	1.61	0.43
1:A:60:LEU:HD12	1:A:60:LEU:HA	1.90	0.43
1:A:88:ALA:O	1:A:92:VAL:HG23	2.18	0.43
1:B:129:ALA:O	1:B:141:LEU:HD13	2.18	0.43
1:B:170:THR:O	1:B:174:LEU:HG	2.19	0.43
1:A:53:GLU:O	1:A:57:GLN:HG2	2.19	0.43
1:B:103:PHE:CD1	1:B:103:PHE:C	2.91	0.43
1:B:63:ILE:HB	1:B:64:PRO:HD3	2.00	0.43
1:B:61:MET:HE3	1:B:61:MET:HB2	1.83	0.42
1:B:88:ALA:N	1:B:89:PRO:HD3	2.33	0.42
1:B:103:PHE:CE1	1:B:265:VAL:HG11	2.54	0.42
1:A:88:ALA:N	1:A:89:PRO:HD3	2.34	0.42
1:B:238:ARG:HA	1:B:238:ARG:HD3	1.87	0.42
1:B:266:ARG:O	1:B:266:ARG:HG2	2.18	0.42
1:A:72:GLU:CD	1:A:72:GLU:H	2.22	0.42
1:B:149:GLN:OE1	1:B:175:ASP:OD1	2.38	0.42
1:A:205:ILE:HG13	1:A:206:TYR:N	2.35	0.41
1:B:47:LEU:HD12	1:B:47:LEU:HA	1.93	0.41
1:B:195:LYS:H	1:B:195:LYS:HG2	1.50	0.41
1:B:177:LEU:HG	1:B:178:MET:CE	2.51	0.41
1:B:149:GLN:HE21	1:B:149:GLN:HB2	1.69	0.40
1:A:49:VAL:HB	1:A:54:PHE:CE2	2.56	0.40
1:A:63:ILE:HB	1:A:64:PRO:HD3	2.03	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	243/271 (90%)	238 (98%)	5 (2%)	0	100	100
1	B	240/271 (89%)	237 (99%)	3 (1%)	0	100	100
All	All	483/542 (89%)	475 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	228/248 (92%)	219 (96%)	9 (4%)	32	35
1	B	227/248 (92%)	206 (91%)	21 (9%)	9	5
All	All	455/496 (92%)	425 (93%)	30 (7%)	16	14

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	107	ARG
1	A	148	LEU
1	A	155	ARG
1	A	182	ASP
1	A	194	LEU
1	A	195	LYS
1	A	257	HIS
1	A	273	LYS
1	B	47	LEU
1	B	52	GLU
1	B	60	LEU
1	B	72	GLU
1	B	83	GLU
1	B	96	ARG
1	B	103	PHE
1	B	116	LYS
1	B	138	LEU

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Mol	Chain	Res	Type
1	B	148	LEU
1	B	180	LYS
1	B	185	LYS
1	B	194	LEU
1	B	195	LYS
1	B	196	MET
1	B	238	ARG
1	B	242	ASP
1	B	251	HIS
1	B	266	ARG
1	B	273	LYS
1	B	285	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	136	ASN
1	A	228	GLN
1	A	257	HIS
1	A	279	ASN
1	B	85	HIS
1	B	149	GLN
1	B	226	ASN
1	B	228	GLN
1	B	279	ASN

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 monosaccharides 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)

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	220:SER	C	221:GLY	N	1.11

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	245/271 (90%)	0.06	8 (3%)	46	46	10, 19, 35, 48	0
1	B	244/271 (90%)	0.02	3 (1%)	79	80	13, 22, 35, 48	0
All	All	489/542 (90%)	0.04	11 (2%)	62	63	10, 20, 35, 48	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	MET	5.0
1	A	196	MET	3.7
1	A	257	HIS	3.0
1	A	219	ALA	3.0
1	B	103	PHE	3.0
1	B	251	HIS	2.7
1	A	220	SER	2.5
1	A	266	ARG	2.4
1	A	264	SER	2.3
1	A	224	MET	2.1
1	A	44	PHE	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 monosaccharides 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.