



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 11:26 AM EDT

PDB ID : 5CSW  
Title : B-RAF IN COMPLEX WITH Dabrafenib  
Authors : Bader, G.; Stadtmüller, H.; Steurer, S.  
Deposited on : 2015-07-23  
Resolution : 2.66 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

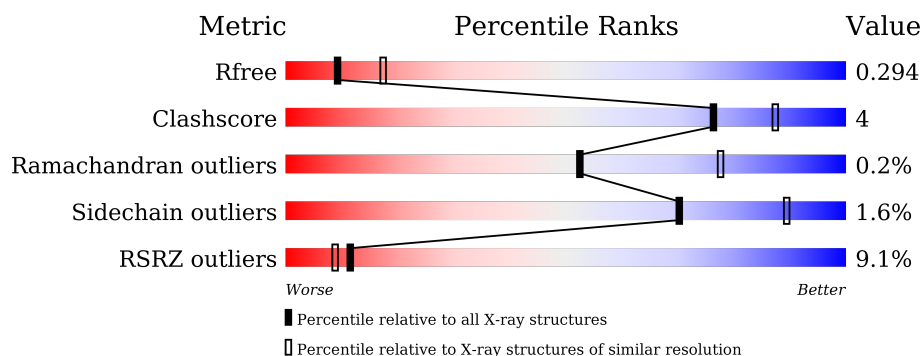
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	282	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>
1	B	282	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4146 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	65	0	0
			2038	1292	363	370	13			
1	B	252	Total	C	N	O	S	94	0	0
			2021	1284	359	366	12			

There are 34 discrepancies between the modelled and reference sequences:

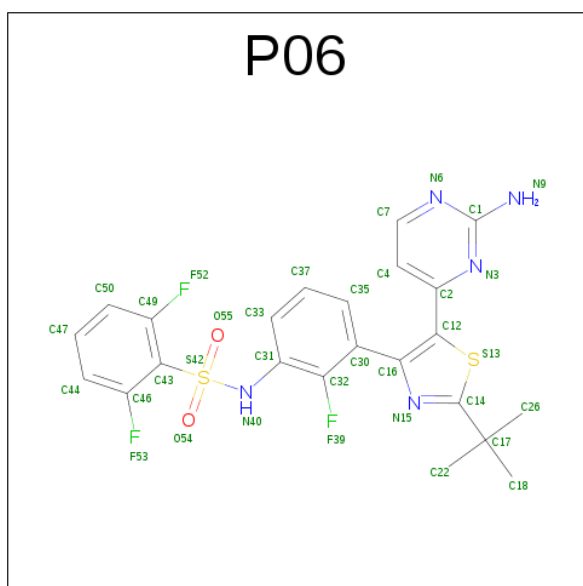
Chain	Residue	Modelled	Actual	Comment	Reference
A	443	PRO	ARG	engineered mutation	UNP P15056
A	543	ALA	ILE	engineered mutation	UNP P15056
A	544	SER	ILE	engineered mutation	UNP P15056
A	551	LYS	ILE	engineered mutation	UNP P15056
A	562	ARG	GLN	engineered mutation	UNP P15056
A	588	ASN	LEU	engineered mutation	UNP P15056
A	630	SER	LYS	engineered mutation	UNP P15056
A	667	GLU	PHE	engineered mutation	UNP P15056
A	673	SER	TYR	engineered mutation	UNP P15056
A	688	ARG	ALA	engineered mutation	UNP P15056
A	706	SER	LEU	engineered mutation	UNP P15056
A	709	ARG	GLN	engineered mutation	UNP P15056
A	713	GLU	SER	engineered mutation	UNP P15056
A	716	GLU	LEU	engineered mutation	UNP P15056
A	720	GLU	SER	engineered mutation	UNP P15056
A	722	SER	-	expression tag	UNP P15056
A	723	GLY	-	expression tag	UNP P15056
B	443	PRO	ARG	engineered mutation	UNP P15056
B	543	ALA	ILE	engineered mutation	UNP P15056
B	544	SER	ILE	engineered mutation	UNP P15056
B	551	LYS	ILE	engineered mutation	UNP P15056
B	562	ARG	GLN	engineered mutation	UNP P15056
B	588	ASN	LEU	engineered mutation	UNP P15056
B	630	SER	LYS	engineered mutation	UNP P15056
B	667	GLU	PHE	engineered mutation	UNP P15056

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Chain	Residue	Modelled	Actual	Comment	Reference
B	673	SER	TYR	engineered mutation	UNP P15056
B	688	ARG	ALA	engineered mutation	UNP P15056
B	706	SER	LEU	engineered mutation	UNP P15056
B	709	ARG	GLN	engineered mutation	UNP P15056
B	713	GLU	SER	engineered mutation	UNP P15056
B	716	GLU	LEU	engineered mutation	UNP P15056
B	720	GLU	SER	engineered mutation	UNP P15056
B	722	SER	-	expression tag	UNP P15056
B	723	GLY	-	expression tag	UNP P15056

- Molecule 2 is Dabrafenib (three-letter code: P06) (formula:  $C_{23}H_{20}F_3N_5O_2S_2$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		
2	B	1	Total	C	F	N	O	S	0	0
			35	23	3	5	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total	Cl	0
			1	1	

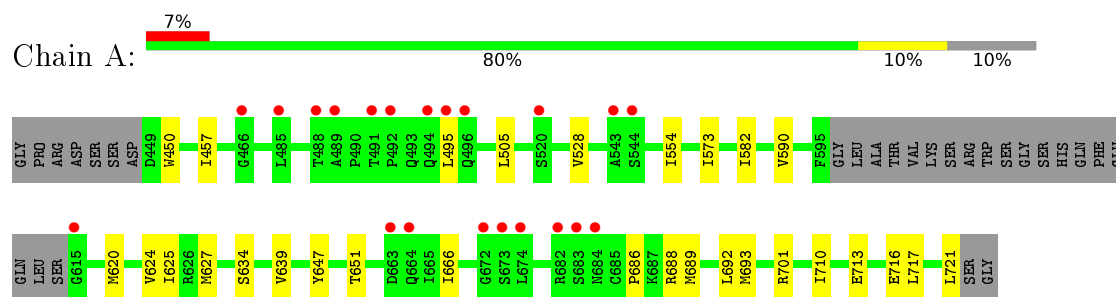
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	7	Total	O	0	0
			7	7		

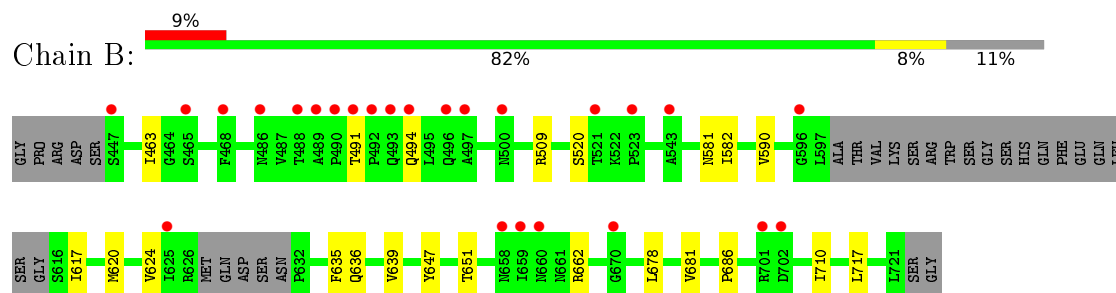
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Serine/threonine-protein kinase B-raf



- Molecule 1: Serine/threonine-protein kinase B-raf



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.36 Å   48.09 Å   101.17 Å 90.00°   95.32°   90.00°	Depositor
Resolution (Å)	100.73 – 2.66 44.30 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.9 (100.73-2.66) 99.9 (44.30-2.66)	Depositor EDS
$R_{merge}$	9.00	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 2.65 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.217   ,   0.282 0.240   ,   0.294	Depositor DCC
$R_{free}$ test set	847 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 16.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16008 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P06, CL

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	0.52	0/2080	0.65	0/2802
1	B	0.51	0/2062	0.64	0/2776
All	All	0.52	0/4142	0.65	0/5578

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2038	0	2055	20	0
1	B	2021	0	2043	11	0
2	A	35	0	20	2	0
2	B	35	0	20	0	0
3	B	1	0	0	0	0
4	A	9	0	0	0	0
4	B	7	0	0	0	0
All	All	4146	0	4138	30	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 4.



All (30) 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:688:ARG:CZ	1:A:713:GLU:OE2	2.39	0.70
1:A:620:MET:CE	1:A:624:VAL:HG12	2.32	0.59
1:A:692:LEU:HD21	1:A:710:ILE:HG23	1.85	0.58
1:A:554:ILE:HD12	1:A:721:LEU:HD22	1.86	0.57
1:B:582:ILE:HG23	1:B:590:VAL:HG13	1.86	0.56
1:B:651:THR:HG22	1:B:681:VAL:HA	1.89	0.53
1:A:457:ILE:HD13	1:A:528:VAL:HG21	1.90	0.53
1:A:620:MET:HE2	1:A:624:VAL:HG12	1.91	0.51
1:A:647:TYR:CZ	1:A:651:THR:HG21	2.46	0.50
1:A:688:ARG:HB2	1:A:717:LEU:HD13	1.94	0.49
1:A:582:ILE:HG23	1:A:590:VAL:HG13	1.96	0.47
1:B:678:LEU:O	1:B:681:VAL:HG22	2.15	0.47
1:A:688:ARG:NH2	1:A:713:GLU:OE2	2.50	0.45
1:A:505:LEU:HD13	2:A:801:P06:C50	2.46	0.45
1:A:639:VAL:HG13	1:A:710:ILE:HD11	1.98	0.45
1:A:573:ILE:HD13	1:A:634:SER:HA	1.99	0.44
1:B:491:THR:HG22	1:B:494:GLN:OE1	2.17	0.44
1:A:505:LEU:HD13	2:A:801:P06:C49	2.48	0.43
1:B:686:PRO:CB	1:B:717:LEU:HD11	2.48	0.43
1:B:620:MET:CE	1:B:624:VAL:HG12	2.49	0.43
1:A:686:PRO:CB	1:A:717:LEU:HD11	2.49	0.42
1:B:635:PHE:O	1:B:639:VAL:HG23	2.20	0.42
1:A:457:ILE:HD13	1:A:528:VAL:CG2	2.50	0.42
1:A:625:ILE:CG2	1:A:666:ILE:HG23	2.50	0.42
1:A:689:MET:O	1:A:693:MET:HE2	2.20	0.42
1:B:647:TYR:CZ	1:B:651:THR:HG21	2.54	0.42
1:B:639:VAL:HG13	1:B:710:ILE:HD11	2.02	0.41
1:A:620:MET:HE2	1:A:624:VAL:CG1	2.50	0.41
1:A:450:TRP:CH2	1:B:509:ARG:HD2	2.56	0.40
1:B:617:ILE:HD11	1:B:662:ARG:HB2	2.04	0.40

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	A	250/282 (89%)	239 (96%)	10 (4%)	1 (0%)	39	65
1	B	246/282 (87%)	235 (96%)	11 (4%)	0	100	100
All	All	496/564 (88%)	474 (96%)	21 (4%)	1 (0%)	52	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	ARG

### 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	A	224/247 (91%)	221 (99%)	3 (1%)	76	91
1	B	222/247 (90%)	218 (98%)	4 (2%)	66	88
All	All	446/494 (90%)	439 (98%)	7 (2%)	70	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	LEU
1	A	627	MET
1	A	716	GLU
1	B	463	ILE
1	B	520	SER
1	B	581	ASN
1	B	636	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	628	GLN
1	B	581	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	P06	A	801	-	33,38,38	0.92	1 (3%)	39,58,58	2.41	9 (23%)
2	P06	B	801	-	33,38,38	0.93	0	39,58,58	2.41	8 (20%)

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
2	P06	A	801	-	-	0/16/25/25	0/4/4/4
2	P06	B	801	-	-	0/16/25/25	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	P06	C1-N9	2.12	1.38	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	P06	N6-C1-N3	-4.30	121.48	125.86
2	B	801	P06	N6-C1-N3	-3.83	121.96	125.86
2	A	801	P06	C4-C7-N6	-3.52	119.76	123.88
2	B	801	P06	C4-C2-N3	-3.29	117.23	121.98
2	B	801	P06	C4-C7-N6	-2.62	120.81	123.88
2	A	801	P06	C4-C2-N3	-2.49	118.38	121.98
2	B	801	P06	O54-S42-N40	2.04	111.81	106.70
2	B	801	P06	C46-C43-C49	2.50	118.40	116.62
2	B	801	P06	C4-C2-C12	3.10	124.55	120.63
2	A	801	P06	N9-C1-N6	3.12	120.26	117.35
2	A	801	P06	O54-S42-O55	3.27	123.88	119.54
2	A	801	P06	C4-C2-C12	3.44	124.98	120.63
2	A	801	P06	C46-C43-C49	3.55	119.16	116.62
2	B	801	P06	C7-N6-C1	3.73	119.61	116.37
2	A	801	P06	C7-N6-C1	4.97	120.68	116.37
2	A	801	P06	C2-N3-C1	10.00	121.18	116.32
2	B	801	P06	C2-N3-C1	11.15	121.74	116.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	P06	2	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	254/282 (90%)	0.53	21 (8%) 14 11	17, 29, 43, 53	19 (7%)
1	B	252/282 (89%)	0.75	25 (9%) 9 7	10, 29, 44, 61	27 (10%)
All	All	506/564 (89%)	0.64	46 (9%) 11 9	10, 29, 43, 61	46 (9%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	SER	5.8
1	B	489	ALA	4.8
1	B	488	THR	4.6
1	B	496	GLN	4.6
1	B	596	GLY	3.9
1	B	521	THR	3.7
1	A	544	SER	3.5
1	B	494	GLN	3.5
1	B	543	ALA	3.5
1	B	491	THR	3.5
1	B	468	PHE	3.3
1	B	500	ASN	3.3
1	B	492	PRO	3.3
1	A	664	GLN	3.2
1	A	496	GLN	3.2
1	B	660	ASN	3.1
1	B	493	GLN	3.1
1	A	684	ASN	3.1
1	B	486	ASN	3.0
1	B	523	PRO	3.0
1	B	497	ALA	2.9
1	B	490	PRO	2.9
1	A	682	ARG	2.7
1	A	663	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	491	THR	2.7
1	A	615	GLY	2.6
1	A	495	LEU	2.6
1	A	672	GLY	2.6
1	A	673	SER	2.6
1	A	492	PRO	2.5
1	A	488	THR	2.4
1	B	447	SER	2.4
1	B	701	ARG	2.3
1	A	489	ALA	2.3
1	A	485	LEU	2.3
1	A	543	ALA	2.2
1	B	659	ILE	2.2
1	A	494	GLN	2.2
1	B	670	GLY	2.2
1	A	520	SER	2.1
1	A	683	SER	2.1
1	B	625	ILE	2.1
1	A	466	GLY	2.0
1	B	658	ASN	2.0
1	B	702	ASP	2.0
1	A	674	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	P06	A	801	35/35	0.93	0.23	0.18	28,40,48,50	0
2	P06	B	801	35/35	0.94	0.23	-0.08	31,40,47,48	0
3	CL	B	802	1/1	0.85	0.23	-	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.