



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:17 pm GMT

PDB ID : 5FD2
Title : B-Raf wild-type kinase domain in complex with a purinylpyridinylamino-based inhibitor
Authors : Whittington, D.A.; Epstein, L.F.
Deposited on : 2015-12-15
Resolution : 2.89 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

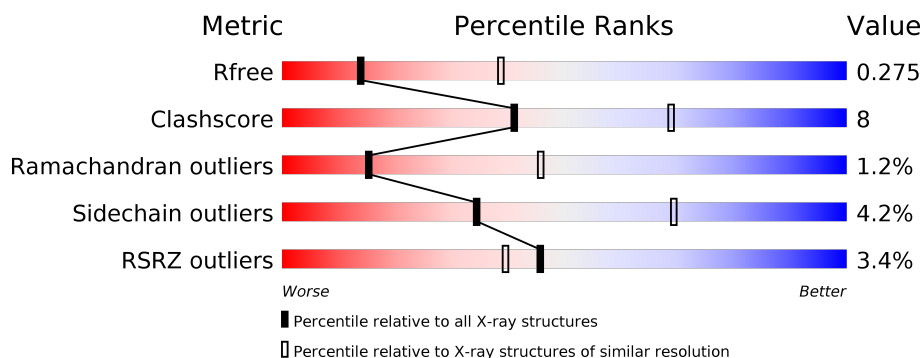
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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. 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	300	
1	B	300	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4072 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.

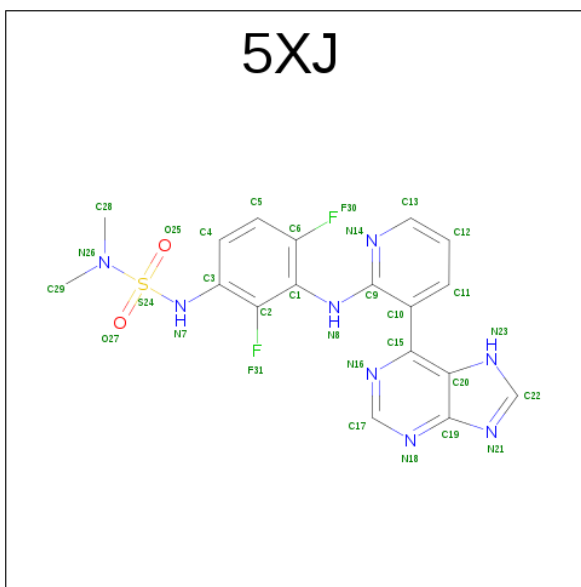
- Molecule 1 is a protein called Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2115	1355	370	377	13			
1	B	234	Total	C	N	O	S	0	0	0
			1863	1195	321	334	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	HIS	-	expression tag	UNP P15056
A	428	HIS	-	expression tag	UNP P15056
A	429	HIS	-	expression tag	UNP P15056
A	430	HIS	-	expression tag	UNP P15056
A	431	HIS	-	expression tag	UNP P15056
A	432	HIS	-	expression tag	UNP P15056
B	427	HIS	-	expression tag	UNP P15056
B	428	HIS	-	expression tag	UNP P15056
B	429	HIS	-	expression tag	UNP P15056
B	430	HIS	-	expression tag	UNP P15056
B	431	HIS	-	expression tag	UNP P15056
B	432	HIS	-	expression tag	UNP P15056

- Molecule 2 is 6-[2-[[3-(dimethylsulfamoylamino)-2,6-bis(fluoranyl)phenyl]amino]pyridin-3-yl]-7 {H}-purine (three-letter code: 5XJ) (formula: C₁₈H₁₆F₂N₈O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			31	18	2	8	2	1		
2	B	1	Total	C	F	N	O	S	0	0
			31	18	2	8	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	2	Total	O	0	0
			2	2		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.79Å 80.09Å 245.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.89 49.63 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.89) 97.6 (49.63-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.278 0.213 , 0.275	Depositor DCC
R_{free} test set	952 reflections (6.18%)	DCC
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	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	0.92	EDS
Total number of atoms	4072	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 4.73% 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: 5XJ

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	0.58	0/2161	0.66	0/2916
1	B	0.50	1/1902 (0.1%)	0.58	0/2568
All	All	0.54	1/4063 (0.0%)	0.62	0/5484

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	619	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

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	A	2115	0	2150	34	0
1	B	1863	0	1853	31	0
2	A	31	0	0	3	0
2	B	31	0	0	2	0
3	A	30	0	0	0	0
3	B	2	0	0	0	0
All	All	4072	0	4003	65	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 (65) 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:498:PHE:CE2	1:B:525:LEU:HD11	2.14	0.83
1:B:518:GLY:O	1:B:528:VAL:HG12	1.85	0.77
1:A:575:ARG:HD2	1:A:598:ALA:HB1	1.72	0.70
1:B:639:VAL:HG13	1:B:710:ILE:HD11	1.75	0.69
1:A:548:PHE:HB2	1:A:553:LEU:HD21	1.76	0.68
1:B:650:MET:HE3	1:B:685:CYS:HB3	1.78	0.63
1:A:712:ALA:HB3	1:B:716:LEU:HD21	1.82	0.61
1:B:514:LEU:HD23	2:B:801:5XJ:C29	2.32	0.59
1:A:484:MET:CE	1:A:524:GLN:OE1	2.51	0.59
1:A:712:ALA:HB3	1:B:716:LEU:CD2	2.34	0.58
1:A:576:ASP:O	1:A:581:ASN:ND2	2.37	0.57
1:B:504:VAL:O	1:B:508:THR:HG23	2.03	0.57
1:A:626:ARG:NH2	1:A:670:GLY:O	2.37	0.56
1:B:642:PHE:CZ	1:B:646:LEU:HD21	2.41	0.56
1:A:484:MET:HE3	1:A:524:GLN:OE1	2.06	0.56
1:A:505:LEU:HD21	1:A:596:GLY:CA	2.36	0.55
1:B:540:HIS:CD2	1:B:584:LEU:HD12	2.40	0.55
1:B:650:MET:HE3	1:B:685:CYS:CB	2.36	0.55
1:A:554:ILE:HG12	1:A:689:MET:HE1	1.89	0.55
1:B:620:MET:HB2	1:B:625:ILE:HD12	1.89	0.54
1:B:582:ILE:HG23	1:B:590:VAL:HG13	1.90	0.54
1:A:505:LEU:HD21	1:A:596:GLY:HA2	1.90	0.54
1:B:454:ASP:N	1:B:454:ASP:OD1	2.41	0.53
1:A:548:PHE:HB2	1:A:553:LEU:CD2	2.37	0.53
1:B:626:ARG:O	1:B:627:MET:C	2.47	0.52
1:A:586:GLU:OE1	1:A:586:GLU:HA	2.10	0.52
2:A:801:5XJ:N8	2:A:801:5XJ:N16	2.57	0.52
1:B:482:VAL:HG22	1:B:528:VAL:HG23	1.91	0.52
1:A:717:LEU:C	1:A:717:LEU:HD12	2.29	0.52
1:A:650:MET:SD	1:A:689:MET:HG2	2.50	0.51
1:A:600:VAL:HG13	1:A:604:TRP:CE3	2.48	0.49
1:B:471:VAL:HG22	1:B:483:LYS:HA	1.95	0.48
1:B:557:ALA:HB2	1:B:649:LEU:CD1	2.43	0.48
1:B:622:PRO:O	1:B:625:ILE:HG22	2.14	0.47
1:A:463:ILE:HD11	1:A:473:LYS:HB2	1.96	0.47
1:A:484:MET:HE2	1:A:524:GLN:OE1	2.14	0.46
1:A:669:VAL:HG23	1:A:674:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:PHE:CG	1:B:525:LEU:HD21	2.51	0.45
1:B:656:TYR:CD1	1:B:674:LEU:HD11	2.52	0.45
1:B:717:LEU:HD12	1:B:717:LEU:O	2.17	0.44
1:A:587:ASP:OD1	1:A:589:THR:N	2.50	0.44
1:B:578:LYS:HG2	1:B:581:ASN:ND2	2.32	0.43
1:A:582:ILE:HG23	1:A:590:VAL:CG1	2.48	0.43
1:A:584:LEU:CD2	1:A:590:VAL:HG22	2.49	0.43
1:B:498:PHE:CD2	1:B:525:LEU:HD21	2.53	0.43
1:A:677:ASP:OD1	1:A:677:ASP:C	2.57	0.43
1:A:647:TYR:CZ	1:A:651:THR:HG21	2.54	0.43
1:B:457:ILE:O	1:B:458:THR:CB	2.66	0.43
1:A:505:LEU:HD13	2:A:801:5XJ:C28	2.49	0.43
1:A:582:ILE:HG23	1:A:590:VAL:HG13	2.00	0.43
1:A:452:ILE:HD12	1:A:528:VAL:HG21	2.01	0.42
1:A:471:VAL:HG21	2:A:801:5XJ:C13	2.49	0.42
1:B:665:ILE:O	1:B:669:VAL:HG23	2.19	0.42
1:B:521:THR:HG23	1:B:521:THR:O	2.20	0.42
1:A:626:ARG:O	1:A:628:GLN:N	2.53	0.42
2:B:801:5XJ:N16	2:B:801:5XJ:N8	2.65	0.42
1:A:552:LYS:O	1:A:556:ILE:HG12	2.19	0.42
1:B:686:PRO:HG2	1:B:717:LEU:HD13	2.02	0.41
1:A:578:LYS:HD2	1:A:580:ASN:HB2	2.03	0.41
1:B:696:CYS:O	1:B:704:ARG:HD2	2.21	0.41
1:A:550:MET:HE3	1:A:685:CYS:HA	2.02	0.41
1:B:717:LEU:HD12	1:B:717:LEU:C	2.41	0.41
1:A:635:PHE:O	1:A:639:VAL:HG23	2.21	0.40
1:B:639:VAL:HG13	1:B:710:ILE:CD1	2.47	0.40
1:A:555:ASP:OD1	1:A:558:ARG:NH1	2.55	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	260/300 (87%)	246 (95%)	12 (5%)	2 (1%)	22	57
1	B	226/300 (75%)	207 (92%)	15 (7%)	4 (2%)	10	34
All	All	486/600 (81%)	453 (93%)	27 (6%)	6 (1%)	15	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	523	PRO
1	A	627	MET
1	B	627	MET
1	A	588	LEU
1	B	594	ASP
1	B	545	GLU

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	232/266 (87%)	221 (95%)	11 (5%)	30	65
1	B	201/266 (76%)	194 (96%)	7 (4%)	41	75
All	All	433/532 (81%)	415 (96%)	18 (4%)	34	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	GLU
1	A	468	PHE
1	A	506	ARG
1	A	551	ILE
1	A	587	ASP
1	A	588	LEU
1	A	614	SER
1	A	623	GLU
1	A	625	ILE
1	A	657	SER

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Mol	Chain	Res	Type
1	A	720	SER
1	B	454	ASP
1	B	498	PHE
1	B	500	ASN
1	B	623	GLU
1	B	625	ILE
1	B	657	SER
1	B	717	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
1	A	581	ASN
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](#)

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	5XJ	A	801	-	29,34,34	2.53	5 (17%)	34,50,50	2.68	12 (35%)
2	5XJ	B	801	-	29,34,34	2.56	5 (17%)	34,50,50	2.69	13 (38%)

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	5XJ	A	801	-	-	0/19/19/19	0/4/4/4
2	5XJ	B	801	-	-	1/19/19/19	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	5XJ	C10-C15	-8.16	1.41	1.49
2	A	801	5XJ	C10-C15	-7.98	1.41	1.49
2	A	801	5XJ	C3-N7	-5.76	1.32	1.42
2	B	801	5XJ	C3-N7	-4.88	1.34	1.42
2	A	801	5XJ	C19-N18	-2.17	1.33	1.37
2	B	801	5XJ	C15-N16	2.52	1.35	1.32
2	A	801	5XJ	O27-S24	5.48	1.49	1.42
2	B	801	5XJ	O25-S24	6.05	1.49	1.42
2	A	801	5XJ	O25-S24	6.13	1.50	1.42
2	B	801	5XJ	O27-S24	6.31	1.50	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	5XJ	O25-S24-O27	-8.21	106.67	119.56
2	A	801	5XJ	N18-C17-N16	-7.97	121.92	128.86
2	B	801	5XJ	N18-C17-N16	-7.00	122.76	128.86
2	A	801	5XJ	O25-S24-O27	-6.86	108.79	119.56
2	B	801	5XJ	C20-C15-N16	-4.73	117.09	123.01
2	A	801	5XJ	C20-C15-N16	-4.51	117.35	123.01
2	B	801	5XJ	C1-N8-C9	-3.47	119.91	124.55
2	B	801	5XJ	C19-C20-N23	-3.36	106.17	109.41
2	A	801	5XJ	C28-N26-C29	-3.18	108.05	114.80
2	A	801	5XJ	C19-C20-N23	-3.08	106.44	109.41
2	B	801	5XJ	C28-N26-C29	-2.90	108.65	114.80
2	A	801	5XJ	C12-C13-N14	-2.05	120.03	123.43
2	B	801	5XJ	C15-C20-C19	2.19	119.38	117.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	5XJ	C10-C15-N16	2.19	119.63	115.54
2	A	801	5XJ	C10-C15-N16	2.26	119.77	115.54
2	B	801	5XJ	C17-N16-C15	2.40	121.55	117.64
2	A	801	5XJ	C17-N16-C15	2.61	121.89	117.64
2	B	801	5XJ	C17-N18-C19	2.67	119.61	113.33
2	A	801	5XJ	C6-C1-C2	2.74	118.55	115.72
2	B	801	5XJ	C6-C1-C2	2.78	118.58	115.72
2	A	801	5XJ	C13-N14-C9	2.86	122.67	116.74
2	A	801	5XJ	C17-N18-C19	2.96	120.29	113.33
2	B	801	5XJ	C10-C9-N8	3.21	124.18	120.22
2	B	801	5XJ	C13-N14-C9	3.23	123.45	116.74
2	A	801	5XJ	F30-C6-C1	5.47	122.40	117.72

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	5XJ	N7-S24-N26-C28

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	5XJ	3	0
2	B	801	5XJ	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 [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	264/300 (88%)	-0.04	1 (0%)	92 92	18, 37, 72, 111	0
1	B	234/300 (78%)	0.53	16 (6%)	18 13	41, 72, 164, 187	0
All	All	498/600 (83%)	0.22	17 (3%)	46 39	18, 53, 147, 187	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	ASP	5.6
1	B	627	MET	4.9
1	B	524	GLN	4.2
1	B	523	PRO	3.9
1	B	484	MET	3.6
1	B	482	VAL	3.4
1	B	527	ILE	2.7
1	A	467	SER	2.6
1	B	525	LEU	2.6
1	B	526	ALA	2.4
1	B	473	LYS	2.2
1	B	533	GLU	2.2
1	B	628	GLN	2.2
1	B	470	THR	2.2
1	B	630	LYS	2.2
1	B	625	ILE	2.1
1	B	498	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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	5XJ	B	801	31/31	0.86	0.26	0.03	59,74,85,90	0
2	5XJ	A	801	31/31	0.97	0.14	-1.56	24,27,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.