



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:20 AM UTC

PDB ID : 6EJN / pdb_00006ejn
Title : The KLC2 TPR domain bound to the JIP3 leucine zipper domain
Authors : Cockburn, J.; Hesketh, S.J.; Way, M.
Deposited on : 2017-09-22
Resolution : 3.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

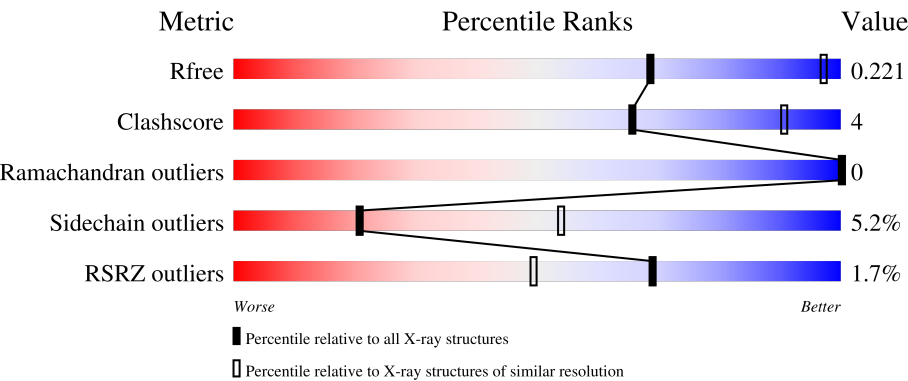
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	291	2% 76% 17% 7%
1	B	291	% 77% 13% 8%
2	C	75	% 69% 11% 20%
2	D	75	% 71% 11% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5207 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 Kinesin light chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2155	1351	389	407	8			
1	B	267	Total	C	N	O	S	0	0	0
			2122	1328	385	401	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	GLY	-	expression tag	UNP Q91YS4
A	190	ARG	-	expression tag	UNP Q91YS4
B	189	GLY	-	expression tag	UNP Q91YS4
B	190	ARG	-	expression tag	UNP Q91YS4

- Molecule 2 is a protein called C-Jun-amino-terminal kinase-interacting protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	60	Total	C	N	O	S	0	0	0
			461	286	81	93	1			
2	D	61	Total	C	N	O	S	0	0	0
			469	292	82	94	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	412	GLY	-	expression tag	UNP Q9ESN9
C	413	PRO	-	expression tag	UNP Q9ESN9
C	414	GLY	-	expression tag	UNP Q9ESN9
C	415	GLY	-	expression tag	UNP Q9ESN9
C	416	ARG	-	expression tag	UNP Q9ESN9
D	412	GLY	-	expression tag	UNP Q9ESN9
D	413	PRO	-	expression tag	UNP Q9ESN9
D	414	GLY	-	expression tag	UNP Q9ESN9

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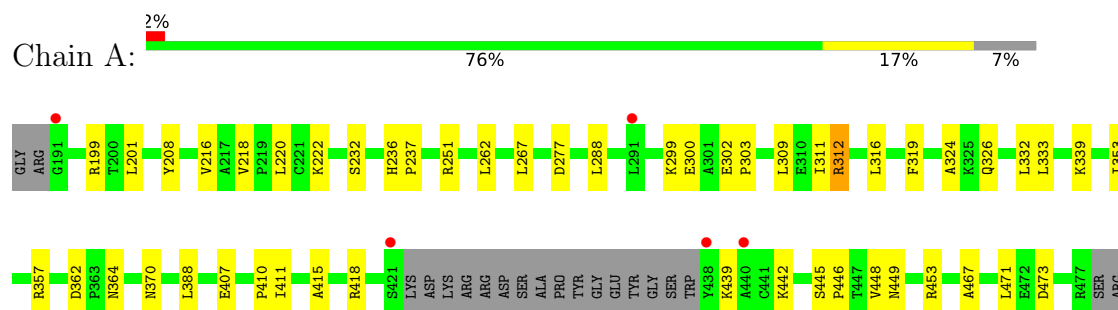
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Chain	Residue	Modelled	Actual	Comment	Reference
D	415	GLY	-	expression tag	UNP Q9ESN9
D	416	ARG	-	expression tag	UNP Q9ESN9

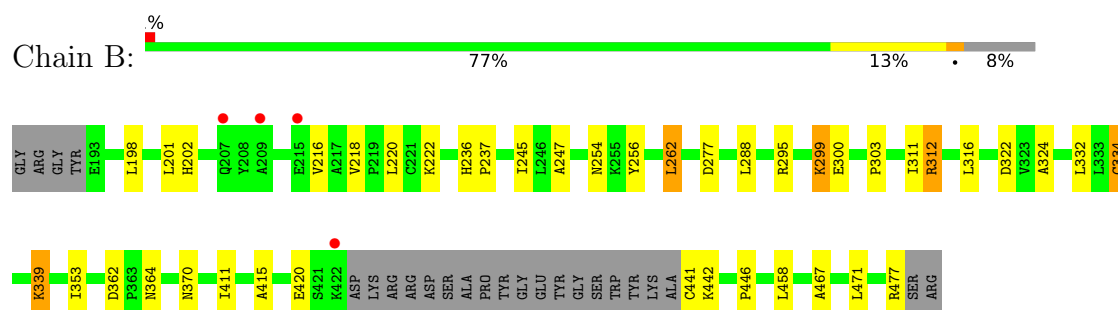
3 Residue-property plots

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.

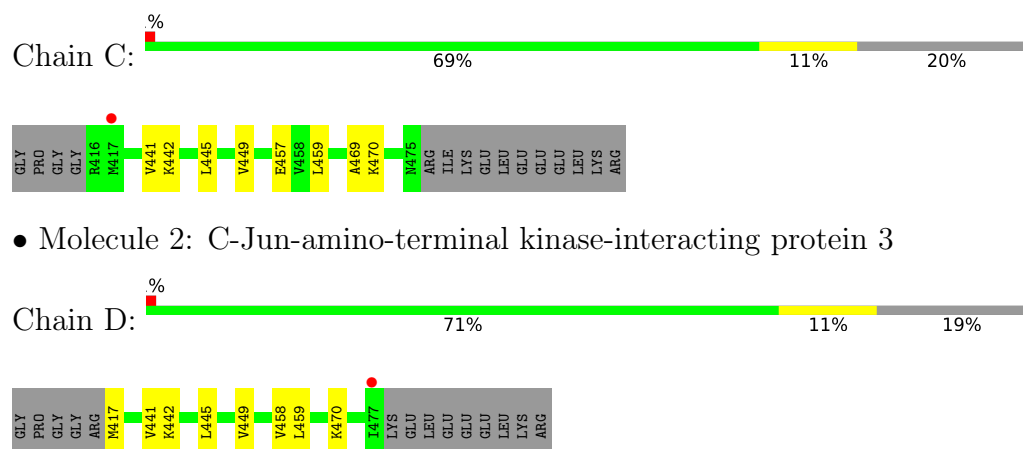
• Molecule 1: Kinesin light chain 2



• Molecule 1: Kinesin light chain 2



• Molecule 2: C-Jun-amino-terminal kinase-interacting protein 3



• Molecule 2: C-Jun-amino-terminal kinase-interacting protein 3

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	163.30Å 163.30Å 77.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.71 – 3.20 67.71 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (67.71-3.20) 99.0 (67.71-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.191 , 0.210 0.201 , 0.221	Depositor DCC
R_{free} test set	967 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	106.4	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 94.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5207	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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	0.82	0/2192	1.51	14/2958 (0.5%)
1	B	0.82	0/2157	1.51	13/2910 (0.4%)
2	C	0.70	0/460	1.47	2/614 (0.3%)
2	D	0.73	0/468	1.46	2/625 (0.3%)
All	All	0.80	0/5277	1.50	31/7107 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	ASP	CA-CB-CG	7.80	120.40	112.60
1	A	407	GLU	N-CA-C	-6.89	100.61	110.59
1	B	441	CYS	CA-C-N	6.71	131.94	122.08
1	B	441	CYS	C-N-CA	6.71	131.94	122.08
1	A	442	LYS	CA-C-N	5.86	127.16	121.65
1	A	442	LYS	C-N-CA	5.86	127.16	121.65
1	A	370	ASN	CA-C-N	5.65	127.79	120.44
1	A	370	ASN	C-N-CA	5.65	127.79	120.44
1	B	339	LYS	CA-C-N	5.62	129.25	120.82
1	B	339	LYS	C-N-CA	5.62	129.25	120.82
1	A	446	PRO	CA-C-N	5.53	127.69	120.28
1	A	446	PRO	C-N-CA	5.53	127.69	120.28
1	A	410	PRO	CA-C-N	5.53	127.52	120.56
1	A	410	PRO	C-N-CA	5.53	127.52	120.56
1	B	370	ASN	CA-C-N	5.48	127.56	120.44
1	B	370	ASN	C-N-CA	5.48	127.56	120.44
1	A	216	VAL	N-CA-C	-5.42	106.90	111.56
1	B	420	GLU	CA-C-N	5.37	131.79	121.54
1	B	420	GLU	C-N-CA	5.37	131.79	121.54
2	D	458	VAL	CA-C-N	5.33	127.42	120.28
2	D	458	VAL	C-N-CA	5.33	127.42	120.28
1	B	216	VAL	N-CA-C	-5.27	107.03	111.56
1	A	339	LYS	CA-C-N	5.24	128.67	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	LYS	C-N-CA	5.24	128.67	120.82
2	C	469	ALA	CA-C-N	5.18	127.17	120.44
2	C	469	ALA	C-N-CA	5.18	127.17	120.44
1	B	446	PRO	CA-C-N	5.08	127.08	120.28
1	B	446	PRO	C-N-CA	5.08	127.08	120.28
1	B	334	CYS	CA-C-N	5.07	127.03	120.44
1	B	334	CYS	C-N-CA	5.07	127.03	120.44
1	A	251	ARG	N-CA-C	-5.05	105.46	110.97

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	2155	0	2163	21	0
1	B	2122	0	2137	18	0
2	C	461	0	489	2	0
2	D	469	0	500	3	0
All	All	5207	0	5289	40	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 (40) 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:415:ALA:HB1	1:A:467:ALA:HA	1.61	0.81
1:B:415:ALA:HB1	1:B:467:ALA:HA	1.78	0.64
1:B:247:ALA:HB2	1:B:262:LEU:HB3	1.85	0.58
1:B:277:ASP:HA	1:B:311:ILE:HG12	1.87	0.56
1:B:236:HIS:CD2	1:B:237:PRO:HD2	2.44	0.52
1:A:277:ASP:HA	1:A:311:ILE:HG12	1.91	0.52
1:A:220:LEU:HD13	2:D:441:VAL:HG21	1.92	0.51
1:B:300:GLU:O	1:B:303:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:HIS:CD2	1:A:237:PRO:HD2	2.45	0.51
1:A:218:VAL:HG12	1:A:222:LYS:HE2	1.92	0.50
1:A:300:GLU:O	1:A:303:PRO:HD2	2.11	0.50
1:A:362:ASP:OD1	1:A:364:ASN:HB2	2.12	0.50
1:B:362:ASP:OD1	1:B:364:ASN:HB2	2.12	0.49
1:B:218:VAL:HG12	1:B:222:LYS:HE2	1.96	0.48
1:A:449:ASN:HB3	1:A:453:ARG:NH1	2.30	0.47
1:A:299:LYS:O	1:A:303:PRO:HD3	2.16	0.46
1:B:334:CYS:HB3	1:B:339:LYS:HB2	1.98	0.45
1:B:442:LYS:HB3	1:B:477:ARG:HG2	1.97	0.45
1:B:324:ALA:HB2	1:B:353:ILE:HB	1.98	0.45
1:A:312:ARG:HG2	1:A:316:LEU:HD12	1.99	0.44
1:A:324:ALA:HB2	1:A:353:ILE:HB	1.99	0.44
1:B:299:LYS:O	1:B:303:PRO:HD3	2.17	0.44
1:B:220:LEU:HD13	2:C:441:VAL:HG21	1.99	0.44
1:B:236:HIS:CG	1:B:237:PRO:HD2	2.53	0.44
2:C:445:LEU:HB3	2:D:445:LEU:HB3	2.00	0.44
1:A:236:HIS:CG	1:A:237:PRO:HD2	2.53	0.44
1:A:445:SER:HB3	1:A:448:VAL:HG23	2.00	0.43
1:B:254:ASN:HA	1:B:256:TYR:CE1	2.54	0.43
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.82	0.43
1:A:319:PHE:O	1:A:357:ARG:HG3	2.19	0.42
1:B:312:ARG:HG2	1:B:316:LEU:HD12	2.01	0.42
1:A:411:ILE:H	1:A:411:ILE:HD12	1.84	0.42
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.90	0.42
1:B:411:ILE:HD12	1:B:411:ILE:H	1.84	0.41
1:B:316:LEU:HD13	1:B:322:ASP:HB2	2.03	0.41
1:A:208:TYR:CE2	2:D:441:VAL:HG22	2.56	0.41
1:A:302:GLU:HA	1:A:333:LEU:HD13	2.02	0.41
1:A:309:LEU:HB2	1:A:326:GLN:HG2	2.02	0.41
1:B:202:HIS:CD2	1:B:245:ILE:HG12	2.56	0.41
1:A:232:SER:HB3	1:A:236:HIS:CG	2.56	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	267/291 (92%)	258 (97%)	9 (3%)	0	100	100
1	B	263/291 (90%)	253 (96%)	10 (4%)	0	100	100
2	C	58/75 (77%)	58 (100%)	0	0	100	100
2	D	59/75 (79%)	59 (100%)	0	0	100	100
All	All	647/732 (88%)	628 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	226/242 (93%)	217 (96%)	9 (4%)	28	61
1	B	224/242 (93%)	214 (96%)	10 (4%)	24	58
2	C	51/63 (81%)	46 (90%)	5 (10%)	7	31
2	D	52/63 (82%)	47 (90%)	5 (10%)	8	32
All	All	553/610 (91%)	524 (95%)	29 (5%)	21	54

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ARG
1	A	201	LEU
1	A	262	LEU
1	A	267	LEU
1	A	288	LEU
1	A	312	ARG
1	A	418	ARG
1	A	439	LYS

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Mol	Chain	Res	Type
1	A	471	LEU
1	B	198	LEU
1	B	201	LEU
1	B	262	LEU
1	B	288	LEU
1	B	295	ARG
1	B	299	LYS
1	B	312	ARG
1	B	332	LEU
1	B	458	LEU
1	B	471	LEU
2	C	442	LYS
2	C	449	VAL
2	C	457	GLU
2	C	459	LEU
2	C	470	LYS
2	D	417	MET
2	D	442	LYS
2	D	449	VAL
2	D	459	LEU
2	D	470	LYS

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

Mol	Chain	Res	Type
1	A	244	ASN
1	A	253	GLN
1	A	287	ASN
1	A	335	GLN
1	A	449	ASN
1	A	462	GLN
1	B	253	GLN
1	B	326	GLN
1	B	449	ASN
2	C	428	ASN
2	C	456	GLN
2	C	475	ASN
2	D	428	ASN
2	D	475	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 oligosaccharides 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	271/291 (93%)	-0.22	5 (1%)	67 48	77, 113, 167, 200	0
1	B	267/291 (91%)	-0.15	4 (1%)	72 52	82, 119, 177, 204	0
2	C	60/75 (80%)	0.13	1 (1%)	69 49	85, 137, 223, 227	0
2	D	61/75 (81%)	-0.21	1 (1%)	70 51	92, 148, 221, 234	0
All	All	659/732 (90%)	-0.16	11 (1%)	69 49	77, 119, 192, 234	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	3.3
1	A	440	ALA	3.1
1	A	291	LEU	2.6
1	B	215	GLU	2.5
1	B	422	LYS	2.5
1	B	209	ALA	2.4
1	A	421	SER	2.3
1	A	438	TYR	2.3
2	C	417	MET	2.2
2	D	477	ILE	2.0
1	B	207	GLN	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 oligosaccharides 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.