



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2025 – 04:07 PM EDT

PDB ID : 9E6W / pdb_00009e6w
Title : NF-kappaB RelA homo-dimer bound to a kappaB site of Cxcl2 gene
Authors : Biswas, T.; Shahabi, S.; Ghosh, G.
Deposited on : 2024-10-31
Resolution : 2.04 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

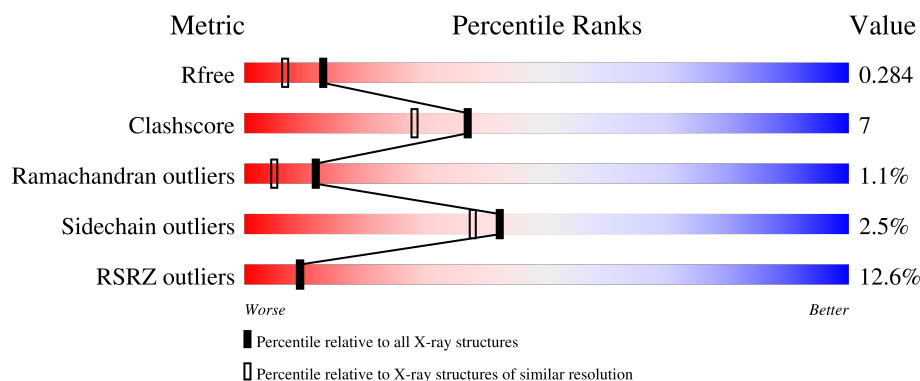
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	287	<div> <div>9%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>
1	B	287	<div> <div>15%</div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>
2	C	18	<div> <div>11%</div> <div>78%</div> <div>22%</div> </div>
3	D	18	<div> <div>17%</div> <div>89%</div> <div>11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5384 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 Transcription factor p65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2197	1369	404	413	11			
1	B	274	Total	C	N	O	S	0	0	0
			2185	1363	402	408	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q04207
B	18	MET	-	initiating methionine	UNP Q04207

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*CP*TP*GP*GP*GP*CP*TP*TP*TP*TP*CP*CP*AP*GP*TP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			369	176	64	111	18			

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*CP*AP*CP*TP*GP*GP*AP*AP*AP*AP*GP*CP*CP*CP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total	C	N	O	P	0	0	0
			369	175	71	105	18			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	113	Total	O	0	0
			113	113		

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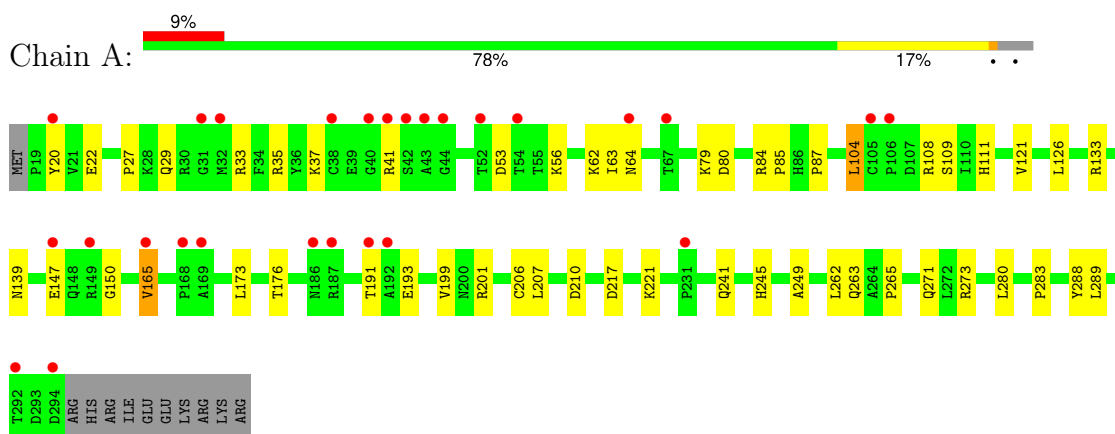
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	22	Total	O	0	0
			22	22		
4	D	26	Total	O	0	0
			26	26		

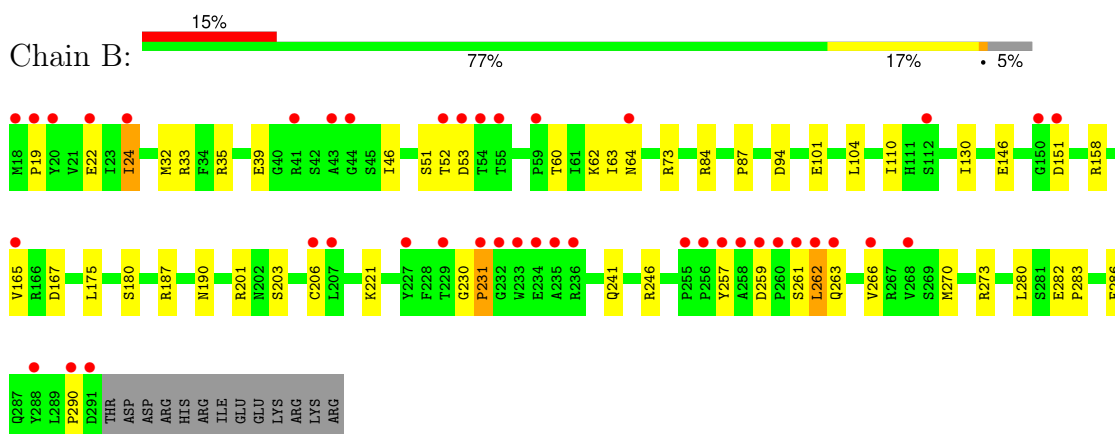
3 Residue-property plots [i](#)

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.

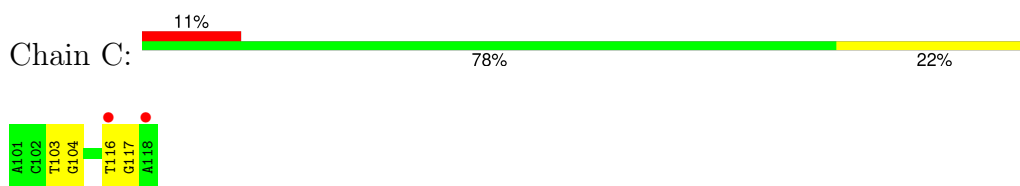
• Molecule 1: Transcription factor p65




• Molecule 1: Transcription factor p65

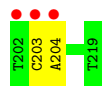


• Molecule 2: DNA (5'-D(P*AP*CP*TP*GP*GP*GP*CP*TP*TP*TP*TP*CP*CP*AP*GP*T P*GP*A)-3')



- Molecule 3: DNA (5'-D(P*TP*CP*AP*CP*TP*GP*GP*AP*AP*AP*AP*GP*CP*CP*CP*AP*GP*T)-3')

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.79Å 133.08Å 45.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.48 – 2.04 37.48 – 2.04	Depositor EDS
% Data completeness (in resolution range)	76.5 (37.48-2.04) 76.6 (37.48-2.04)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_4788	Depositor
R, R_{free}	0.244 , 0.283 0.248 , 0.284	Depositor DCC
R_{free} test set	1752 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	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	0.91	EDS
Total number of atoms	5384	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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](#)

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	0.16	0/2250	0.36	0/3053
1	B	0.14	0/2238	0.37	0/3036
2	C	0.22	0/411	0.46	0/630
3	D	0.23	0/414	0.43	0/636
All	All	0.16	0/5313	0.38	0/7355

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 [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	2197	0	2153	33	0
1	B	2185	0	2148	33	0
2	C	369	0	206	2	0
3	D	369	0	202	1	0
4	A	103	0	0	7	0
4	B	113	0	0	6	0
4	C	22	0	0	0	0
4	D	26	0	0	0	0
All	All	5384	0	4709	68	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 7.

All (68) 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:139:ASN:ND2	4:A:406:HOH:O	2.27	0.67
1:A:62:LYS:HE3	1:A:64:ASN:HD21	1.58	0.67
1:B:206:CYS:SG	4:B:484:HOH:O	2.53	0.66
1:A:165:VAL:O	1:A:173:LEU:N	2.29	0.65
1:A:53:ASP:O	1:A:56:LYS:NZ	2.31	0.62
1:B:63:ILE:HD13	1:B:104:LEU:HD21	1.82	0.61
1:A:108:ARG:NH1	4:A:416:HOH:O	2.35	0.60
1:B:273:ARG:HG3	1:B:280:LEU:HD23	1.84	0.59
1:A:217:ASP:OD1	1:B:246:ARG:NH2	2.36	0.58
1:A:263:GLN:NE2	4:A:417:HOH:O	2.36	0.57
1:B:246:ARG:NH1	4:B:412:HOH:O	2.37	0.56
1:A:199:VAL:HG12	1:A:201:ARG:H	1.70	0.56
1:B:273:ARG:NH2	4:B:413:HOH:O	2.39	0.55
1:B:262:LEU:O	1:B:263:GLN:HB3	2.08	0.54
1:A:265:PRO:HB3	1:A:289:LEU:HD23	1.91	0.52
1:A:37:LYS:HG3	1:A:41:ARG:HH12	1.75	0.52
1:A:85:PRO:HD3	1:A:139:ASN:ND2	2.25	0.51
1:A:33:ARG:HD2	1:A:35:ARG:HH21	1.75	0.51
2:C:103:DT:H2"	2:C:104:DG:C8	2.46	0.50
1:A:84:ARG:NH1	1:A:150:GLY:H	2.09	0.50
1:B:19:PRO:HB3	1:B:64:ASN:O	2.12	0.49
1:A:87:PRO:HB2	1:A:121:VAL:HG11	1.95	0.49
1:A:221:LYS:HD2	1:A:241:GLN:HB3	1.94	0.49
1:A:133:ARG:NH2	4:A:408:HOH:O	2.30	0.49
1:A:273:ARG:HG3	1:A:280:LEU:HG	1.95	0.49
1:A:41:ARG:NE	4:A:414:HOH:O	2.34	0.48
1:A:206:CYS:HB3	1:A:262:LEU:HD12	1.96	0.48
1:B:190:ASN:O	4:B:401:HOH:O	2.20	0.48
1:B:221:LYS:HD2	1:B:241:GLN:HB3	1.96	0.47
1:A:84:ARG:HD3	1:A:147:GLU:O	2.15	0.47
1:B:282:GLU:HG3	1:B:283:PRO:HD2	1.95	0.47
1:B:32:MET:HE1	1:B:46:ILE:HG12	1.95	0.47
1:A:41:ARG:HD2	1:A:41:ARG:HA	1.71	0.47
1:B:270:MET:HE2	1:B:286:PHE:HB2	1.98	0.46
1:B:39:GLU:OE2	1:B:187:ARG:NH2	2.48	0.46
2:C:116:DT:H2"	2:C:117:DG:C8	2.50	0.46
1:B:33:ARG:HB2	1:B:187:ARG:HG3	1.98	0.46
1:A:245:HIS:HB3	1:A:249:ALA:HB3	1.98	0.45
1:B:94:ASP:OD2	4:B:402:HOH:O	2.20	0.45
1:A:27:PRO:O	4:A:401:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ILE:HG13	1:B:60:THR:OG1	2.16	0.44
1:A:20:TYR:CE1	1:A:64:ASN:HB2	2.52	0.44
1:A:104:LEU:HB3	1:A:111:HIS:CE1	2.53	0.44
3:D:203:DC:H2"	3:D:204:DA:C5	2.51	0.44
1:A:84:ARG:HH12	1:A:150:GLY:H	1.64	0.44
1:A:210:ASP:OD2	4:A:402:HOH:O	2.21	0.44
1:B:262:LEU:HD12	1:B:262:LEU:HA	1.82	0.43
1:B:257:TYR:C	1:B:259:ASP:H	2.26	0.43
1:A:22:GLU:O	1:A:62:LYS:N	2.36	0.43
1:B:201:ARG:HD2	1:B:203:SER:O	2.19	0.42
1:B:290:PRO:HA	4:B:484:HOH:O	2.20	0.42
1:A:271:GLN:HB3	1:A:283:PRO:HA	2.02	0.42
1:B:87:PRO:HD3	1:B:130:ILE:HD11	2.01	0.42
1:A:79:LYS:HG2	1:A:80:ASP:OD1	2.20	0.42
1:B:158:ARG:NH1	1:B:180:SER:O	2.52	0.42
1:B:24:ILE:HD13	1:B:62:LYS:HB3	2.01	0.42
1:B:84:ARG:NH2	1:B:151:ASP:O	2.41	0.41
1:B:146:GLU:OE1	1:B:146:GLU:N	2.42	0.41
1:A:63:ILE:O	1:A:109:SER:HB2	2.20	0.41
1:B:259:ASP:C	1:B:261:SER:H	2.28	0.41
1:B:230:GLY:O	1:B:231:PRO:C	2.63	0.41
1:A:265:PRO:HA	1:A:288:TYR:O	2.21	0.41
1:B:263:GLN:H	1:B:290:PRO:HB3	1.86	0.41
1:B:257:TYR:CE2	1:B:266:VAL:HG21	2.56	0.40
1:B:19:PRO:O	1:B:175:LEU:HD22	2.21	0.40
1:B:73:ARG:HB2	1:B:101:GLU:HG3	2.03	0.40
1:A:37:LYS:HG3	1:A:41:ARG:NH1	2.34	0.40
1:B:22:GLU:HB3	1:B:62:LYS:HG2	2.02	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	274/287 (96%)	262 (96%)	11 (4%)	1 (0%)	30	23
1	B	272/287 (95%)	257 (94%)	10 (4%)	5 (2%)	7	2
All	All	546/574 (95%)	519 (95%)	21 (4%)	6 (1%)	12	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	52	THR
1	B	262	LEU
1	B	53	ASP
1	A	29	GLN
1	B	231	PRO
1	B	165	VAL

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	245/257 (95%)	238 (97%)	7 (3%)	37	32
1	B	244/257 (95%)	239 (98%)	5 (2%)	50	47
All	All	489/514 (95%)	477 (98%)	12 (2%)	42	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	126	LEU
1	A	165	VAL
1	A	176	THR
1	A	191	THR
1	A	193	GLU
1	A	207	LEU
1	B	24	ILE
1	B	35	ARG
1	B	51	SER

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Mol	Chain	Res	Type
1	B	110	ILE
1	B	167	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	64	ASN
1	A	111	HIS
1	A	137	ASN
1	A	181	HIS
1	A	263	GLN
1	A	271	GLN
1	B	29	GLN
1	B	58	HIS
1	B	64	ASN
1	B	114	GLN
1	B	119	GLN

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	117:DG	O3'	118:DA	P	2.91

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	276/287 (96%)	0.72	27 (9%) 14 15	14, 30, 50, 89	0
1	B	274/287 (95%)	0.85	42 (15%) 6 6	13, 30, 60, 75	0
2	C	18/18 (100%)	0.97	2 (11%) 12 12	23, 49, 90, 101	0
3	D	18/18 (100%)	0.78	3 (16%) 5 4	24, 40, 93, 97	0
All	All	586/610 (96%)	0.79	74 (12%) 9 9	13, 31, 61, 101	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	SER	8.4
1	B	258	ALA	8.2
1	A	294	ASP	5.8
1	B	150	GLY	5.1
1	A	54	THR	4.6
1	B	262	LEU	4.2
1	A	32	MET	4.2
1	B	44	GLY	3.9
1	B	256	PRO	3.9
1	B	18	MET	3.8
1	A	40	GLY	3.8
1	B	233	TRP	3.7
1	B	55	THR	3.7
1	A	187	ARG	3.7
1	A	168	PRO	3.6
1	B	52	THR	3.6
1	A	41	ARG	3.6
1	A	43	ALA	3.4
1	A	292	THR	3.4
1	A	231	PRO	3.4
1	B	41	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	118	DA	3.2
1	B	291	ASP	3.2
1	A	64	ASN	3.1
3	D	202	DT	3.1
1	B	206	CYS	3.1
1	B	165	VAL	3.0
1	B	257	TYR	3.0
1	B	229	THR	2.9
1	B	259	ASP	2.9
1	B	266	VAL	2.8
1	B	227	TYR	2.8
1	B	290	PRO	2.8
1	B	268	VAL	2.8
3	D	204	DA	2.7
1	B	260	PRO	2.7
1	B	232	GLY	2.7
1	B	24	ILE	2.7
1	A	31	GLY	2.6
1	A	52	THR	2.6
1	A	169	ALA	2.6
1	B	151	ASP	2.6
1	A	149	ARG	2.6
1	B	207	LEU	2.5
1	B	235	ALA	2.5
1	B	54	THR	2.5
1	B	255	PRO	2.5
1	B	64	ASN	2.5
1	B	231	PRO	2.4
1	B	236	ARG	2.4
1	A	186	ASN	2.4
1	A	67	THR	2.4
1	A	20	TYR	2.4
1	B	263	GLN	2.4
1	A	192	ALA	2.4
1	A	106	PRO	2.4
1	A	147	GLU	2.3
1	B	234	GLU	2.3
2	C	116	DT	2.3
1	B	112	SER	2.3
3	D	203	DC	2.3
1	A	44	GLY	2.3
1	B	288	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	165	VAL	2.2
1	A	38	CYS	2.2
1	A	191	THR	2.2
1	B	261	SER	2.1
1	B	20	TYR	2.1
1	B	59	PRO	2.1
1	B	19	PRO	2.0
1	B	43	ALA	2.0
1	A	105	CYS	2.0
1	B	22	GLU	2.0
1	B	53	ASP	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.