wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 01:58 AM EDT

PDB ID	:	4E3C
Title	:	X-ray crystal structure of human IKK2 in an active conformation
Authors	:	Polley, S.; Huang, D.B.; Hauenstein, A.V.; Ghosh, G.; Huxford, T.
Deposited on	:	2012-03-09
Resolution	:	3.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

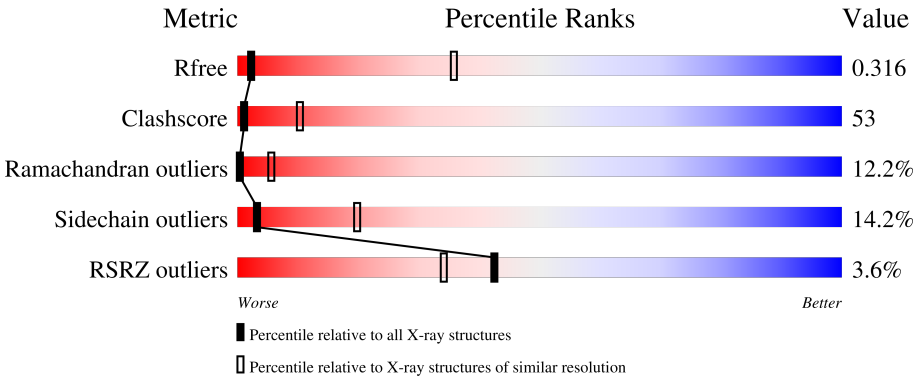
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.98 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	1039 (4.26-3.70)
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RSRZ outliers	127900	1021 (4.30-3.66)

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	669	4% 28% 49% 14% • 7%
1	B	669	3% 28% 48% 17% • 6%
1	C	669	2% 28% 48% 16% • 7%
1	D	669	3% 28% 50% 14% • 7%
1	E	669	4% 27% 51% 14% • 7%

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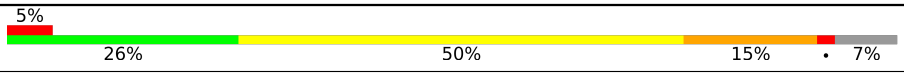
Mol	Chain	Length	Quality of chain
1	F	669	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 30416 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 Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	B	632	Total	C	N	O	S	0	0	0
			5116	3219	904	959	34			
1	C	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	D	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	E	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	F	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	expression tag	UNP O14920
A	2	LEU	-	expression tag	UNP O14920
A	3	TYR	-	expression tag	UNP O14920
A	4	PHE	-	expression tag	UNP O14920
A	5	GLN	-	expression tag	UNP O14920
A	6	GLY	-	expression tag	UNP O14920
A	7	ALA	-	expression tag	UNP O14920
A	8	MET	-	expression tag	UNP O14920
A	9	GLY	-	expression tag	UNP O14920
A	10	SER	-	expression tag	UNP O14920
A	177	GLU	SER	engineered mutation	UNP O14920
A	181	GLU	SER	engineered mutation	UNP O14920
B	1	ASN	-	expression tag	UNP O14920
B	2	LEU	-	expression tag	UNP O14920
B	3	TYR	-	expression tag	UNP O14920
B	4	PHE	-	expression tag	UNP O14920
B	5	GLN	-	expression tag	UNP O14920

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	GLY	-	expression tag	UNP O14920
B	7	ALA	-	expression tag	UNP O14920
B	8	MET	-	expression tag	UNP O14920
B	9	GLY	-	expression tag	UNP O14920
B	10	SER	-	expression tag	UNP O14920
B	177	GLU	SER	engineered mutation	UNP O14920
B	181	GLU	SER	engineered mutation	UNP O14920
C	1	ASN	-	expression tag	UNP O14920
C	2	LEU	-	expression tag	UNP O14920
C	3	TYR	-	expression tag	UNP O14920
C	4	PHE	-	expression tag	UNP O14920
C	5	GLN	-	expression tag	UNP O14920
C	6	GLY	-	expression tag	UNP O14920
C	7	ALA	-	expression tag	UNP O14920
C	8	MET	-	expression tag	UNP O14920
C	9	GLY	-	expression tag	UNP O14920
C	10	SER	-	expression tag	UNP O14920
C	177	GLU	SER	engineered mutation	UNP O14920
C	181	GLU	SER	engineered mutation	UNP O14920
D	1	ASN	-	expression tag	UNP O14920
D	2	LEU	-	expression tag	UNP O14920
D	3	TYR	-	expression tag	UNP O14920
D	4	PHE	-	expression tag	UNP O14920
D	5	GLN	-	expression tag	UNP O14920
D	6	GLY	-	expression tag	UNP O14920
D	7	ALA	-	expression tag	UNP O14920
D	8	MET	-	expression tag	UNP O14920
D	9	GLY	-	expression tag	UNP O14920
D	10	SER	-	expression tag	UNP O14920
D	177	GLU	SER	engineered mutation	UNP O14920
D	181	GLU	SER	engineered mutation	UNP O14920
E	1	ASN	-	expression tag	UNP O14920
E	2	LEU	-	expression tag	UNP O14920
E	3	TYR	-	expression tag	UNP O14920
E	4	PHE	-	expression tag	UNP O14920
E	5	GLN	-	expression tag	UNP O14920
E	6	GLY	-	expression tag	UNP O14920
E	7	ALA	-	expression tag	UNP O14920
E	8	MET	-	expression tag	UNP O14920
E	9	GLY	-	expression tag	UNP O14920
E	10	SER	-	expression tag	UNP O14920
E	177	GLU	SER	engineered mutation	UNP O14920

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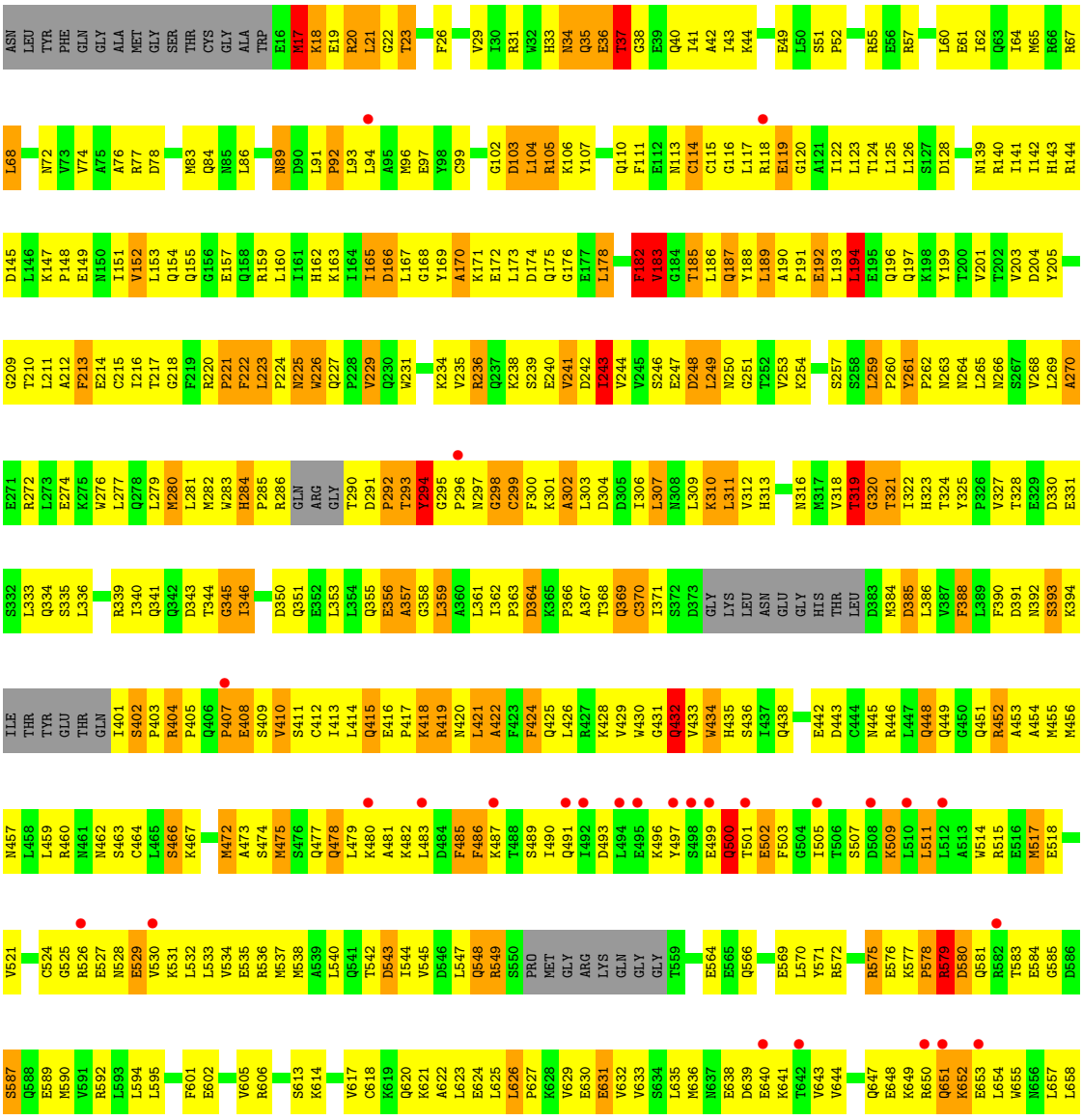
Chain	Residue	Modelled	Actual	Comment	Reference
E	181	GLU	SER	engineered mutation	UNP O14920
F	1	ASN	-	expression tag	UNP O14920
F	2	LEU	-	expression tag	UNP O14920
F	3	TYR	-	expression tag	UNP O14920
F	4	PHE	-	expression tag	UNP O14920
F	5	GLN	-	expression tag	UNP O14920
F	6	GLY	-	expression tag	UNP O14920
F	7	ALA	-	expression tag	UNP O14920
F	8	MET	-	expression tag	UNP O14920
F	9	GLY	-	expression tag	UNP O14920
F	10	SER	-	expression tag	UNP O14920
F	177	GLU	SER	engineered mutation	UNP O14920
F	181	GLU	SER	engineered mutation	UNP O14920

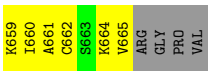
3 Residue-property plots (i)

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.

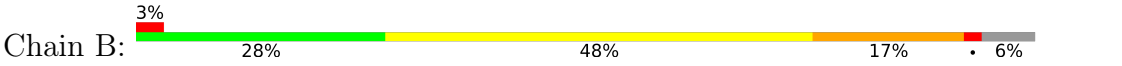
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

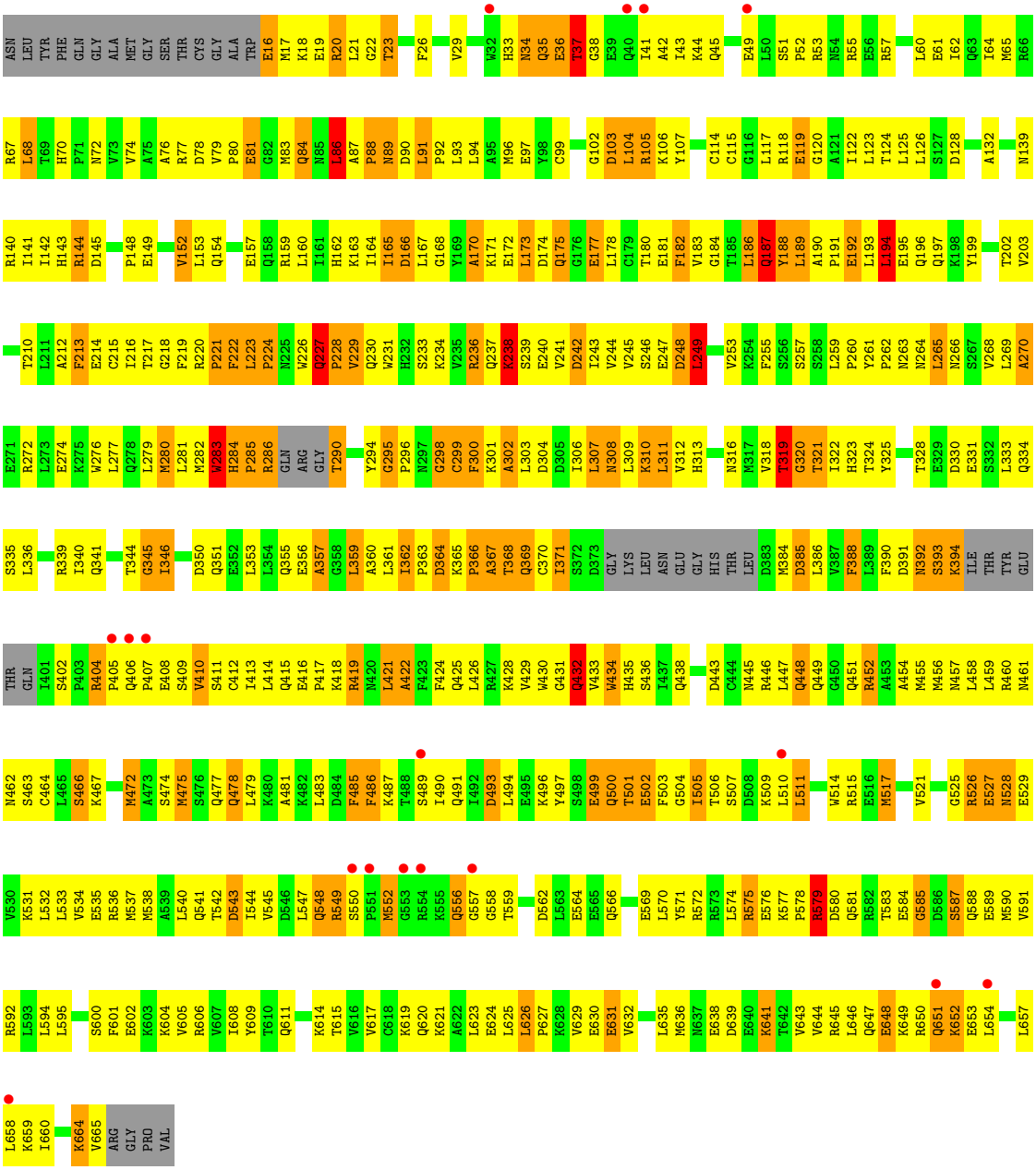
Chain A:



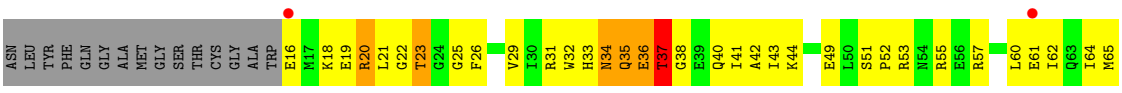


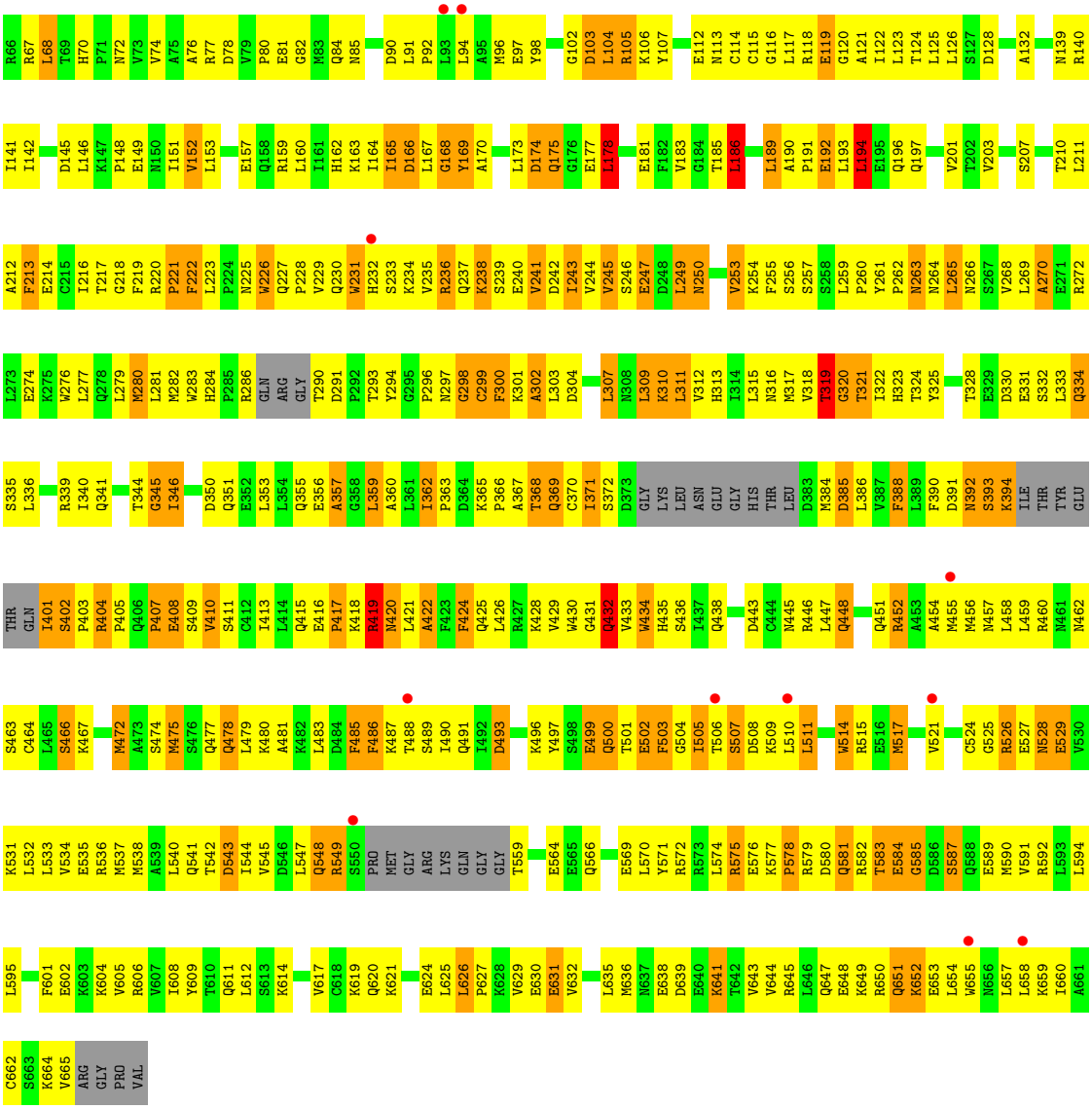
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta





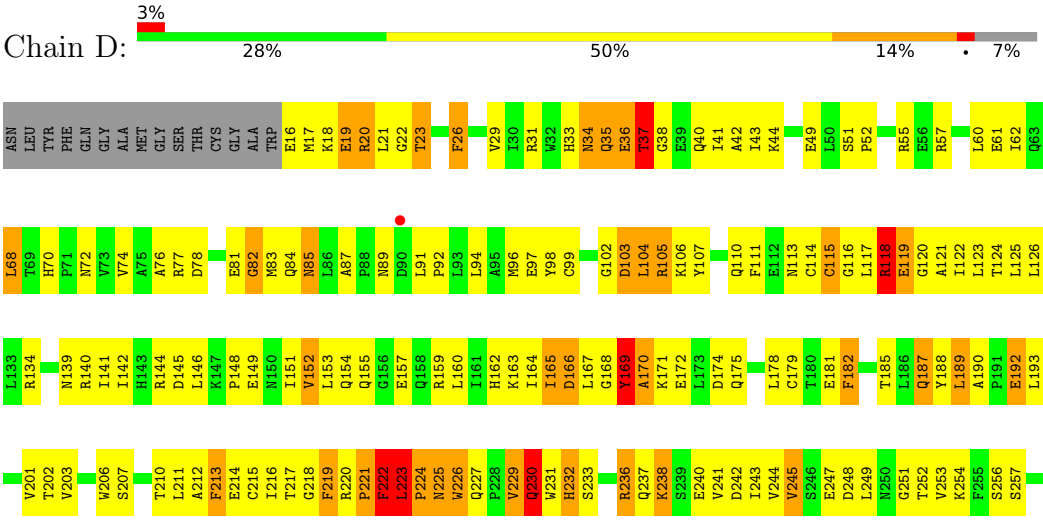
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

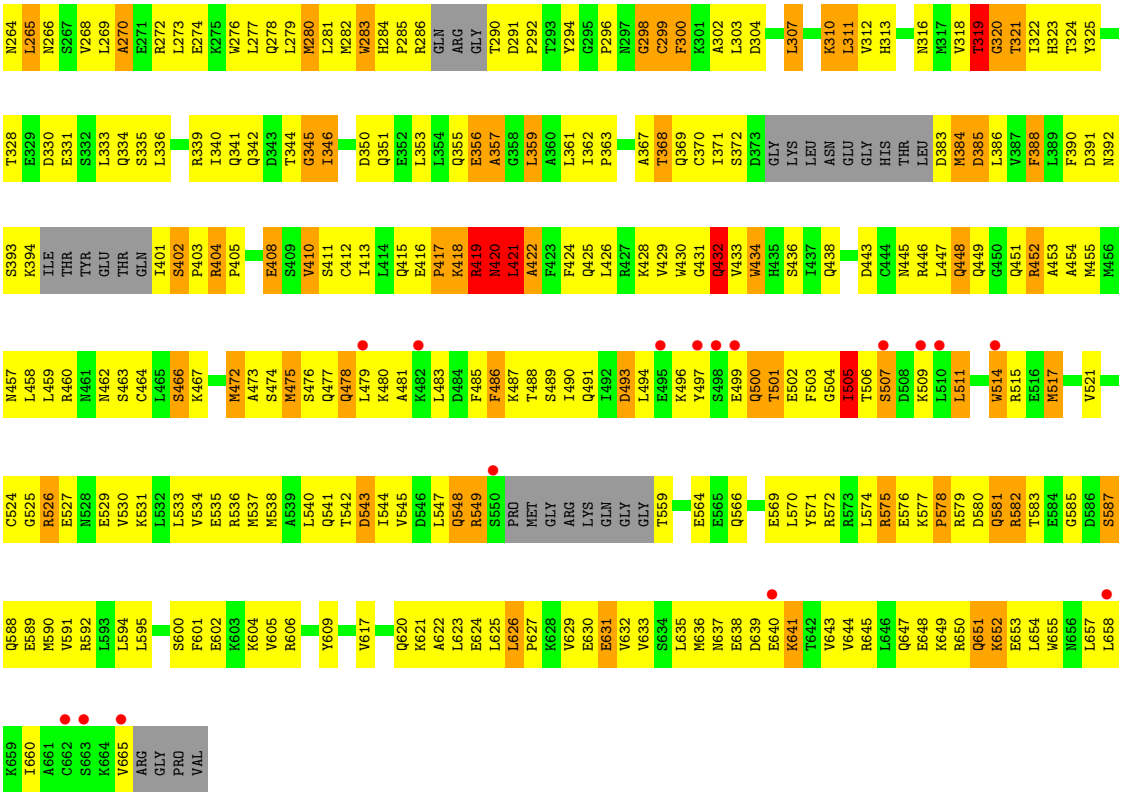




• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

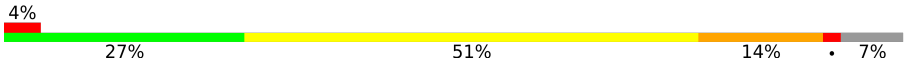
Chain D:

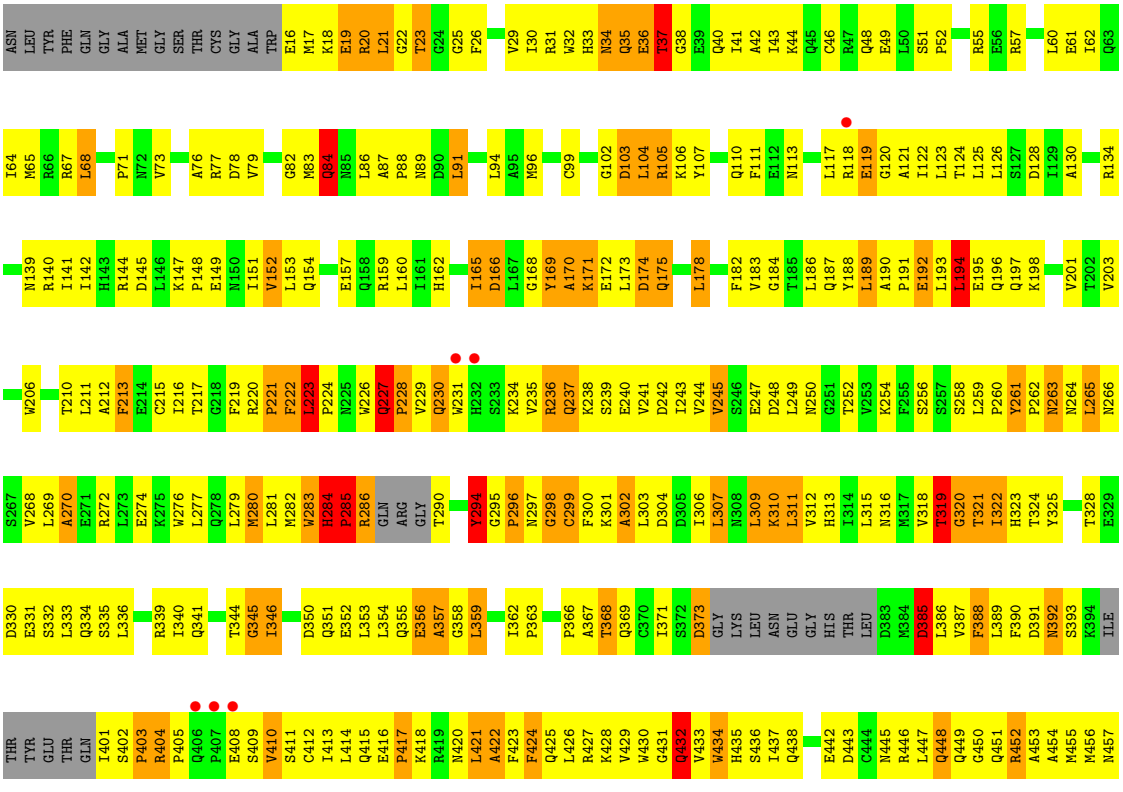


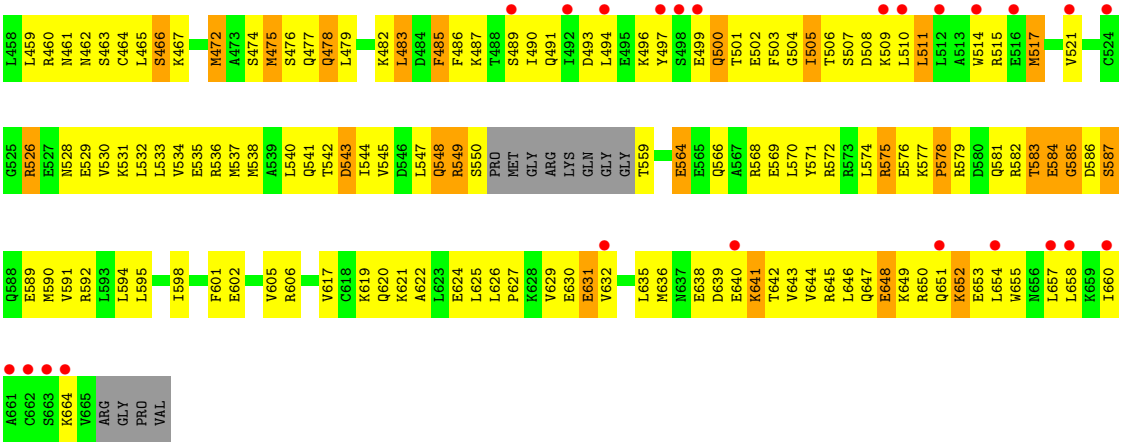


• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain E:

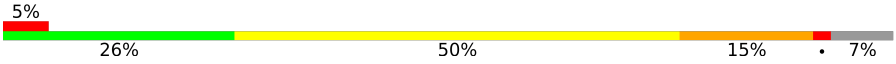


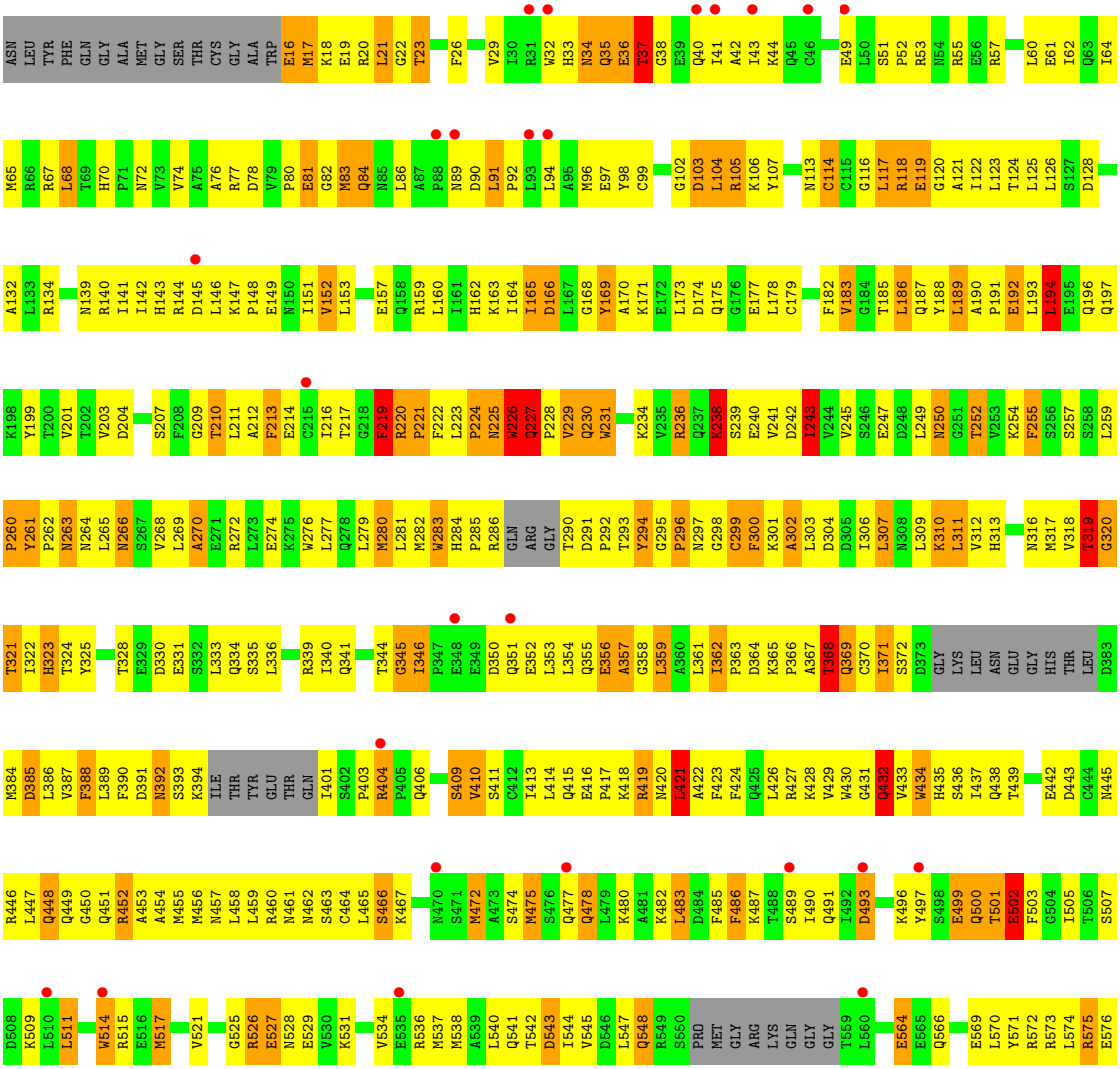


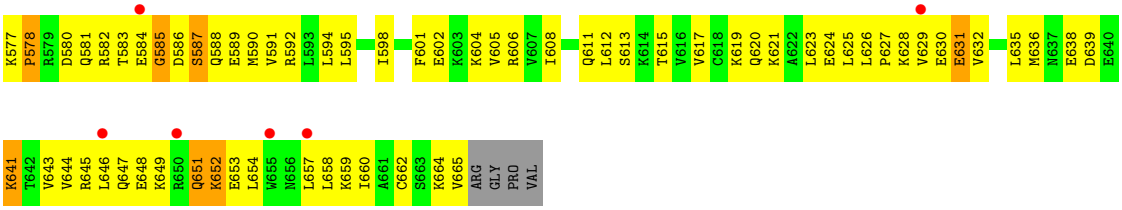


• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain F:






K577 P578 R579 D580 Q581 R582 T583 E584 G585 D586 S587 Q588 E589 M590 V591 R592 L593 L594 L595 I598 F601 E602 K603 K604 V605 R606 V607 I608 Q611 L612 S613 K614 T615 V616 V617 C618 K619 Q620 K621 A622 L623 E624 L625 L626 P627 K628 V629 E630 E631 V632 L635 M636 N637 E638 D639 E640
K641 T642 V643 V644 R645 L646 Q647 E648 K649 R650 Q651 K652 E653 L654 W655 N656 L657 L658 K659 I660 A661 C662 S663 K664 V665 ARG GLY PRO VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	170.81Å 170.81Å 509.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.98 49.73 – 3.97	Depositor EDS
% Data completeness (in resolution range)	81.0 (29.84-3.98) 88.5 (49.73-3.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 4.00Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.267 , 0.299 0.285 , 0.316	Depositor DCC
R_{free} test set	2388 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å^2)	113.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 155.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	30416	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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

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	0.47	0/5142	0.61	3/6937 (0.0%)
1	B	0.47	0/5200	0.69	3/7014 (0.0%)
1	C	0.44	0/5142	0.58	0/6937
1	D	0.45	0/5142	0.69	3/6937 (0.0%)
1	E	0.44	0/5142	0.57	0/6937
1	F	0.42	0/5142	0.57	0/6937
All	All	0.45	0/30910	0.62	9/41699 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	118	ARG	NE-CZ-NH1	-21.84	109.38	120.30
1	D	118	ARG	NE-CZ-NH2	21.77	131.18	120.30
1	B	144	ARG	NE-CZ-NH1	-20.91	109.84	120.30
1	B	144	ARG	NE-CZ-NH2	19.92	130.26	120.30
1	D	118	ARG	CD-NE-CZ	9.85	137.39	123.60

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	5060	0	5109	581	0
1	B	5116	0	5169	569	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5060	0	5109	522	0
1	D	5060	0	5109	557	0
1	E	5060	0	5107	554	0
1	F	5060	0	5107	584	0
All	All	30416	0	30710	3237	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 53.

The worst 5 of 3237 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:419:ARG:NH1	1:B:419:ARG:HB2	1.55	1.18
1:B:366:PRO:HB2	1:B:368:THR:HG23	1.29	1.14
1:C:496:LYS:HE2	1:C:654:LEU:HD21	1.20	1.14
1:F:626:LEU:H	1:F:627:PRO:HD2	1.13	1.13
1:D:479:LEU:HD11	1:D:641:LYS:HG2	1.28	1.11

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	614/669 (92%)	427 (70%)	112 (18%)	75 (12%)	0 5
1	B	624/669 (93%)	411 (66%)	133 (21%)	80 (13%)	0 5
1	C	614/669 (92%)	423 (69%)	117 (19%)	74 (12%)	0 6
1	D	614/669 (92%)	421 (69%)	119 (19%)	74 (12%)	0 6
1	E	614/669 (92%)	417 (68%)	121 (20%)	76 (12%)	0 5
1	F	614/669 (92%)	421 (69%)	120 (20%)	73 (12%)	0 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3694/4014 (92%)	2520 (68%)	722 (20%)	452 (12%)	0 5

5 of 452 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	35	GLN
1	A	92	PRO
1	A	166	ASP
1	A	182	PHE

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	567/601 (94%)	491 (87%)	76 (13%)	4 21
1	B	572/601 (95%)	485 (85%)	87 (15%)	3 17
1	C	567/601 (94%)	490 (86%)	77 (14%)	3 21
1	D	567/601 (94%)	488 (86%)	79 (14%)	3 20
1	E	567/601 (94%)	492 (87%)	75 (13%)	4 21
1	F	567/601 (94%)	478 (84%)	89 (16%)	2 16
All	All	3407/3606 (94%)	2924 (86%)	483 (14%)	3 20

5 of 483 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	559	THR
1	F	388	PHE
1	D	421	LEU
1	F	334	GLN
1	F	564	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	432	GLN
1	D	225	ASN
1	F	500	GLN
1	F	263	ASN
1	C	457	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	624/669 (93%)	0.31	27 (4%)	35	29	56, 129, 201, 287	0
1	B	632/669 (94%)	0.16	17 (2%)	54	44	56, 130, 204, 256	0
1	C	624/669 (93%)	0.11	13 (2%)	63	54	64, 133, 201, 267	0
1	D	624/669 (93%)	0.13	17 (2%)	54	44	62, 132, 201, 286	0
1	E	624/669 (93%)	0.26	30 (4%)	30	25	63, 134, 205, 264	0
1	F	624/669 (93%)	0.25	31 (4%)	28	25	64, 144, 206, 256	0
All	All	3752/4014 (93%)	0.20	135 (3%)	42	34	56, 133, 204, 287	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	510	LEU	9.0
1	A	505	ILE	7.2
1	A	497	TYR	6.3
1	A	495	GLU	5.9
1	D	665	VAL	5.9

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.