



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:47 AM UTC

PDB ID : 3JUA / pdb_00003jua
Title : Structural basis of YAP recognition by TEAD4 in the Hippo pathway
Authors : Chen, L.; Song, H.
Deposited on : 2009-09-15
Resolution : 3.00 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 ⓘ 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:

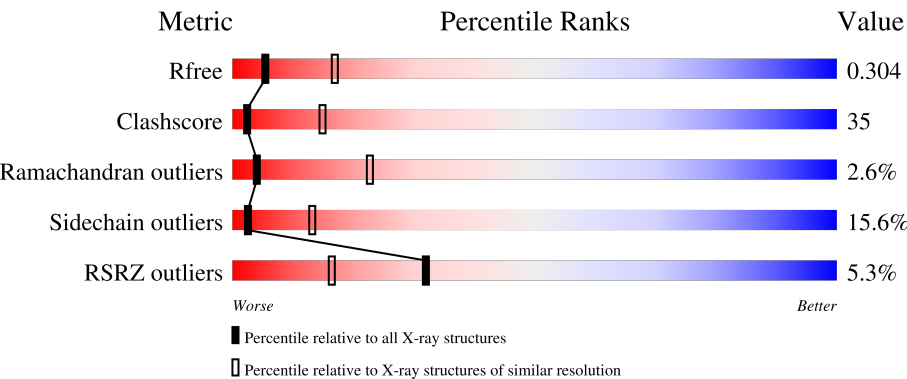
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	220	45% 40% 6% 7%
1	C	220	4% 55% 31% 9%
1	E	220	4% 49% 35% 12%
1	G	220	6% 47% 28% 9% 14%
2	B	39	8% 21% 59% 18%

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Mol	Chain	Length	Quality of chain
2	D	39	5% 46% 28% 13% • 10%
2	F	39	26% 31% 51% 5% 5% 8%
2	H	39	8% 18% 10% 18% • 51%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8055 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 Transcriptional enhancer factor TEF-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	0	0
			1692	1092	281	309	10			
1	C	213	Total	C	N	O	S	0	0	0
			1762	1131	293	328	10			
1	E	216	Total	C	N	O	S	0	0	0
			1782	1144	294	334	10			
1	G	190	Total	C	N	O	S	0	0	0
			1586	1021	263	292	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	SER	-	expression tag	UNP Q62296
A	209	MET	-	expression tag	UNP Q62296
C	208	SER	-	expression tag	UNP Q62296
C	209	MET	-	expression tag	UNP Q62296
E	208	SER	-	expression tag	UNP Q62296
E	209	MET	-	expression tag	UNP Q62296
G	208	SER	-	expression tag	UNP Q62296
G	209	MET	-	expression tag	UNP Q62296

- Molecule 2 is a protein called 65 kDa Yes-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	S	0	0	0
			311	200	52	57	2			
2	D	35	Total	C	N	O	S	0	0	0
			279	180	48	49	2			
2	F	36	Total	C	N	O	S	0	0	0
			286	185	49	50	2			
2	H	19	Total	C	N	O	S	0	0	0
			158	105	28	24	1			

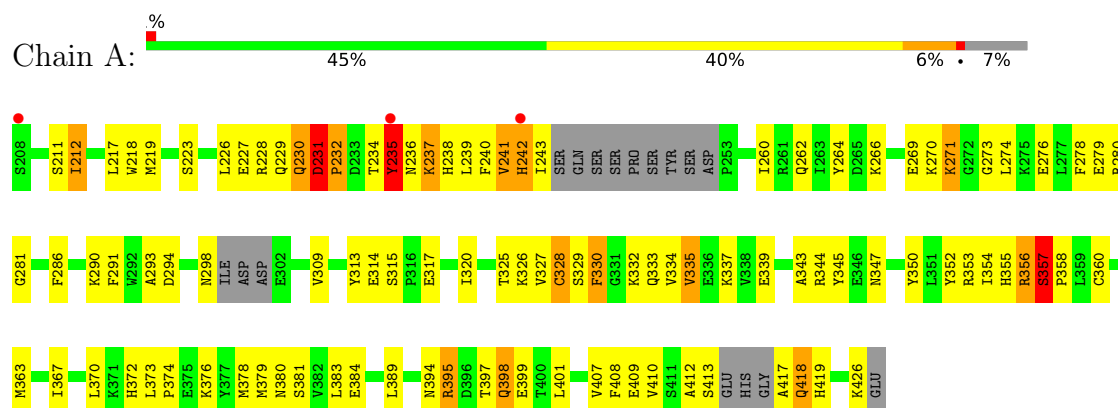
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	7	Total 7	O 7	0	0
3	C	45	Total 45	O 45	0	0
3	D	6	Total 6	O 6	0	0
3	E	51	Total 51	O 51	0	0
3	F	7	Total 7	O 7	0	0
3	G	42	Total 42	O 42	0	0

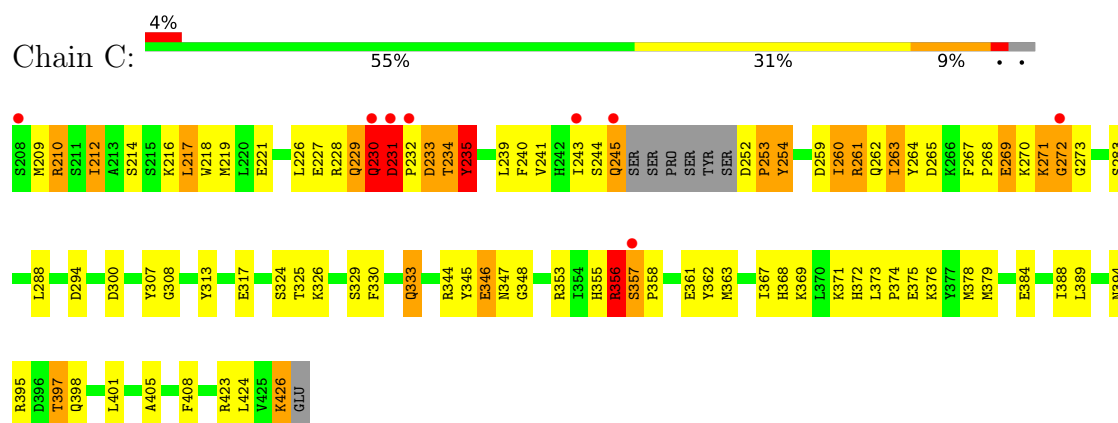
3 Residue-property plots [i](#)

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.

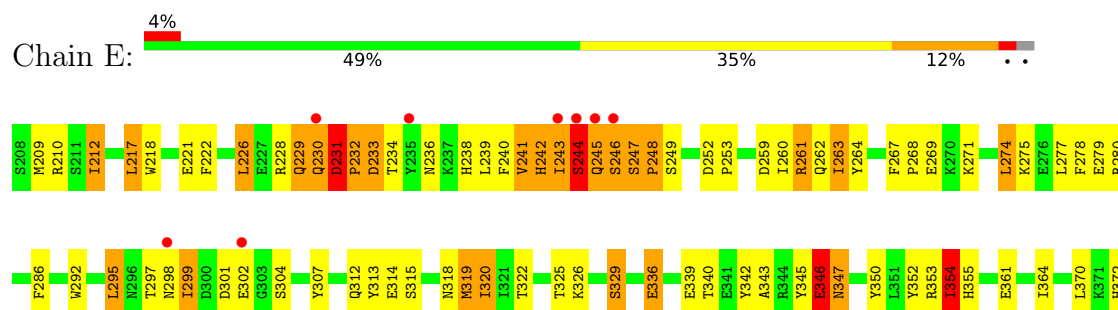
• Molecule 1: Transcriptional enhancer factor TEF-3

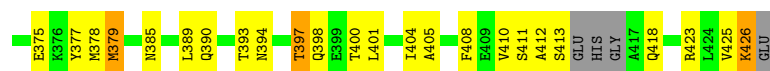


• Molecule 1: Transcriptional enhancer factor TEF-3

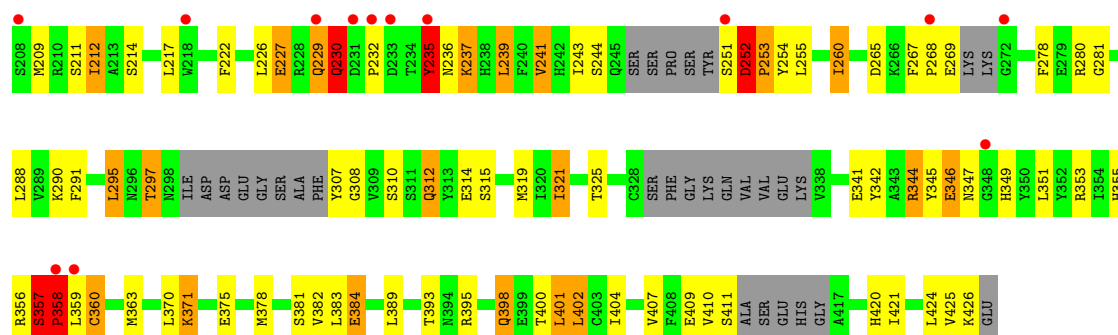


• Molecule 1: Transcriptional enhancer factor TEF-3

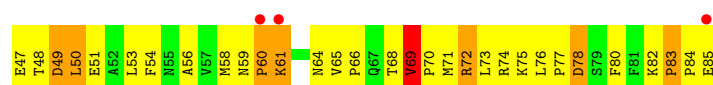




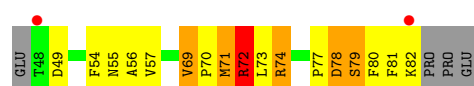
• Molecule 1: Transcriptional enhancer factor TEF-3



• Molecule 2: 65 kDa Yes-associated protein



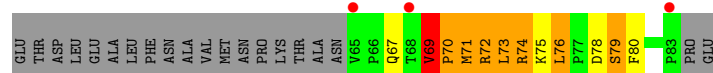
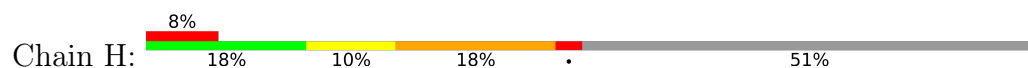
• Molecule 2: 65 kDa Yes-associated protein



• Molecule 2: 65 kDa Yes-associated protein



• Molecule 2: 65 kDa Yes-associated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.98Å 146.91Å 165.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.00) 99.5 (20.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.236 , 0.288 0.255 , 0.304	Depositor DCC
R_{free} test set	3103 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8055	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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	0.69	0/1733	0.97	3/2335 (0.1%)
1	C	0.75	0/1806	1.27	20/2438 (0.8%)
1	E	0.76	2/1827 (0.1%)	1.21	14/2468 (0.6%)
1	G	0.62	1/1623 (0.1%)	1.21	11/2189 (0.5%)
2	B	0.64	0/319	1.13	6/434 (1.4%)
2	D	0.86	1/285 (0.4%)	1.34	2/386 (0.5%)
2	F	0.93	1/293 (0.3%)	1.30	4/398 (1.0%)
2	H	0.65	0/163	1.62	5/220 (2.3%)
All	All	0.72	5/8049 (0.1%)	1.19	65/10868 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
1	E	0	1
1	G	0	1
2	F	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	72	ARG	CA-C	-6.13	1.47	1.53
2	D	72	ARG	N-CA	-5.44	1.40	1.46
1	E	354	ILE	CA-CB	-5.33	1.47	1.54
1	E	248	PRO	CA-C	-5.19	1.46	1.52
1	G	357	SER	CA-C	-5.07	1.46	1.52

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	357	SER	C-N-CD	-19.15	78.46	120.60
1	G	346	GLU	N-CA-C	-15.99	86.74	109.29
1	E	248	PRO	N-CA-C	-14.14	91.11	111.33
1	G	230	GLN	N-CA-C	-12.68	83.78	110.80
2	H	72	ARG	N-CA-C	-12.07	95.56	110.41

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	357	SER	Peptide
1	C	229	GLN	Peptide
1	C	231	ASP	Peptide
1	C	357	SER	Peptide
1	E	229	GLN	Peptide

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	1692	0	1657	127	0
1	C	1762	0	1710	106	0
1	E	1782	0	1730	119	0
1	G	1586	0	1537	98	0
2	B	311	0	315	29	0
2	D	279	0	289	34	0
2	F	286	0	296	28	0
2	H	158	0	170	30	0
3	A	41	0	0	3	0
3	B	7	0	0	3	0
3	C	45	0	0	10	0
3	D	6	0	0	3	0
3	E	51	0	0	6	0
3	F	7	0	0	1	0
3	G	42	0	0	9	0
All	All	8055	0	7704	546	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 35.

The worst 5 of 546 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)
2:H:69:VAL:HG12	2:H:70:PRO:CD	1.54	1.38
1:G:252:ASP:CB	1:G:253:PRO:HD3	1.30	1.37
2:H:75:LYS:O	2:H:76:LEU:HD23	1.18	1.32
1:C:210:ARG:HD3	1:C:252:ASP:OD1	1.27	1.25
2:H:75:LYS:C	2:H:76:LEU:HD23	1.62	1.24

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	196/220 (89%)	173 (88%)	16 (8%)	7 (4%)	2	16
1	C	209/220 (95%)	189 (90%)	18 (9%)	2 (1%)	12	45
1	E	212/220 (96%)	189 (89%)	16 (8%)	7 (3%)	3	17
1	G	178/220 (81%)	164 (92%)	10 (6%)	4 (2%)	5	26
2	B	37/39 (95%)	32 (86%)	4 (11%)	1 (3%)	4	22
2	D	33/39 (85%)	30 (91%)	3 (9%)	0	100	100
2	F	34/39 (87%)	25 (74%)	8 (24%)	1 (3%)	3	20
2	H	17/39 (44%)	10 (59%)	5 (29%)	2 (12%)	0	1
All	All	916/1036 (88%)	812 (89%)	80 (9%)	24 (3%)	4	23

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	231	ASP

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Mol	Chain	Res	Type
1	A	271	LYS
1	C	358	PRO
1	E	244	SER

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	188/203 (93%)	163 (87%)	25 (13%)	4	18
1	C	196/203 (97%)	167 (85%)	29 (15%)	3	15
1	E	200/203 (98%)	168 (84%)	32 (16%)	2	12
1	G	178/203 (88%)	151 (85%)	27 (15%)	3	14
2	B	36/36 (100%)	28 (78%)	8 (22%)	1	5
2	D	32/36 (89%)	25 (78%)	7 (22%)	1	5
2	F	33/36 (92%)	28 (85%)	5 (15%)	3	14
2	H	19/36 (53%)	14 (74%)	5 (26%)	0	3
All	All	882/956 (92%)	744 (84%)	138 (16%)	2	13

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	269	GLU
1	G	321	ILE
1	G	402	LEU
1	C	283	SER
1	C	271	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	229	GLN
1	G	420	HIS

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Mol	Chain	Res	Type
1	G	284	ASN
1	G	368	HIS
1	C	236	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	204/220 (92%)	-0.25	3 (1%) 72 49	15, 25, 35, 43	0
1	C	213/220 (96%)	-0.07	8 (3%) 44 24	18, 28, 39, 53	0
1	E	216/220 (98%)	0.04	8 (3%) 45 25	19, 28, 40, 60	0
1	G	190/220 (86%)	0.33	13 (6%) 23 12	14, 28, 39, 43	0
2	B	39/39 (100%)	0.37	3 (7%) 19 10	21, 25, 36, 36	0
2	D	35/39 (89%)	0.09	2 (5%) 29 15	25, 28, 37, 39	0
2	F	36/39 (92%)	1.38	10 (27%) 1 1	26, 32, 39, 39	0
2	H	19/39 (48%)	0.99	3 (15%) 5 3	21, 27, 34, 34	0
All	All	952/1036 (91%)	0.10	50 (5%) 32 16	14, 28, 39, 60	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	65	VAL	5.5
1	G	231	ASP	5.1
1	E	244	SER	5.1
2	F	61	LYS	5.0
1	G	359	LEU	3.9

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.