



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TVR
Title : HIV-1 RT/9-CL TIBO
Authors : Das, K.; Ding, J.; Hsiou, Y.; Arnold, E.
Deposited on : 1996-04-16
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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

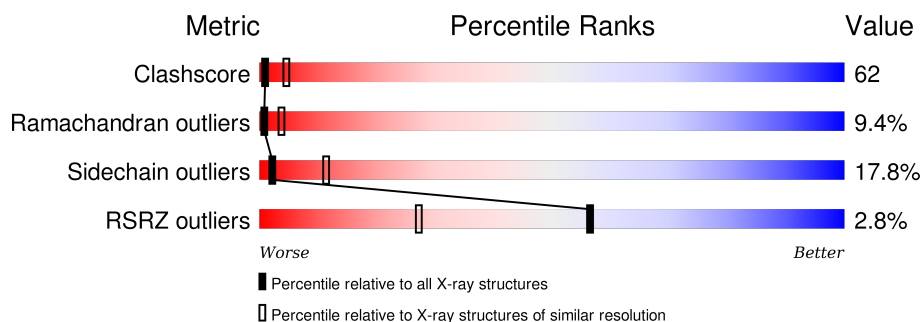
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	558	
2	B	427	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TB9	A	600	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7845 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 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4382	2832	727	817	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

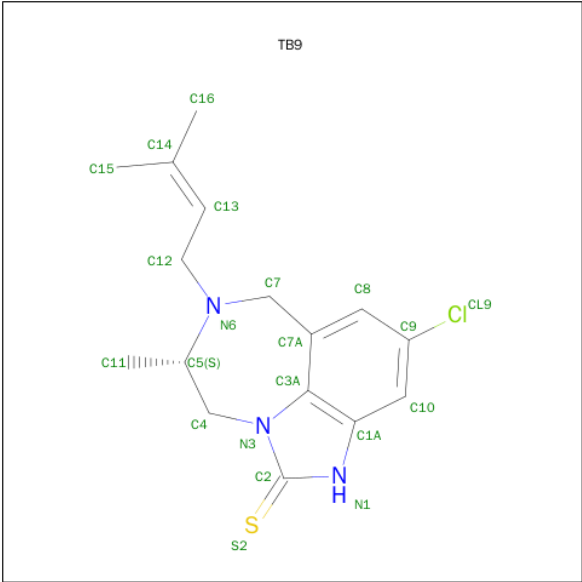
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3442	2240	567	630	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is 4-CHLORO-8-METHYL-7-(3-METHYL-BUT-2-ENYL)-6,7,8,9-TETRAHYDRO-2H-2,7,9A-TRIAZA-BENZO[CD]AZULENE-1-THIONE (three-letter code: TB9) (formula: C₁₆H₂₀ClN₃S).

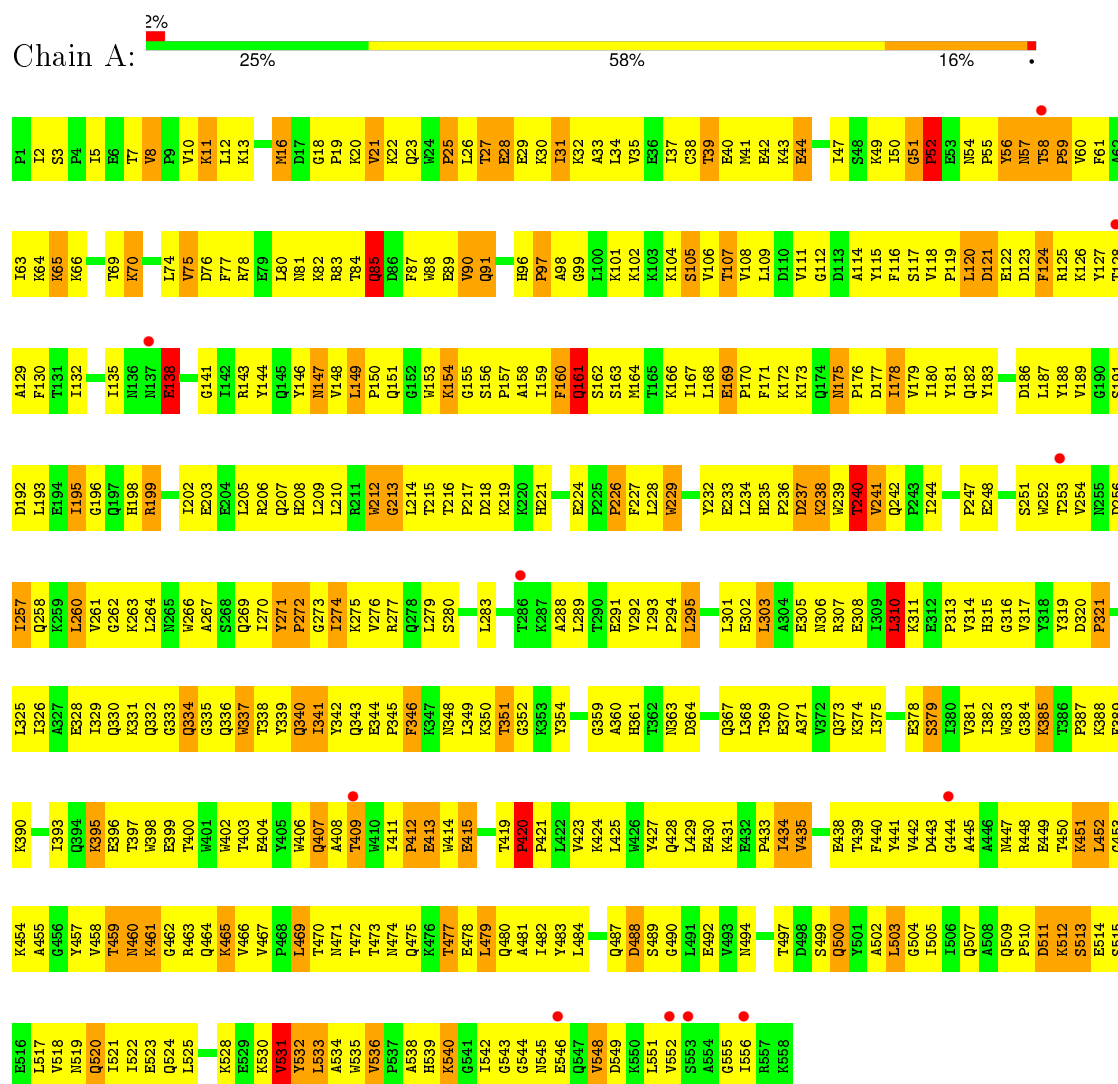


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	S		
3	A	1	21	16	1	3	1	0	0

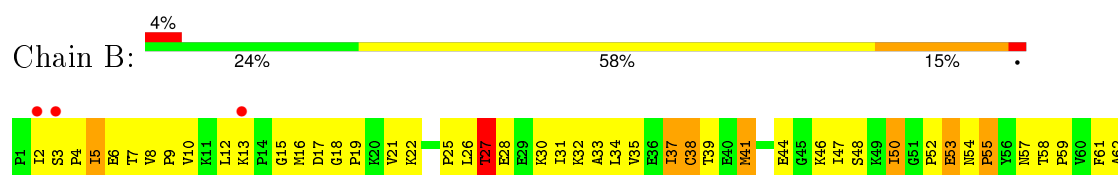
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: REVERSE TRANSCRIPTASE



• Molecule 2: REVERSE TRANSCRIPTASE



E378	S379	I380	V381	I382	I383	F389	K390	L391	P392	I393	Q394	K395	E396	T397	E398	E399	T400	W401	W402	T403	E404	Y405	W406	Q407	P412	E413	W414	E415	E416	V417	M418	T419	P420	P421	L422	V423	K424	L425	W426	Y427																		
Y317	Y318	Y319	D320	P321	S322	K323	D324	L325	A327	E328	I329	Q330	K331	Q332	G333	Q334	G335	Q336	W337	T338	Y339	Q340	I341	Y342	Q343	E344	P345	F346	K347	I348	L349	K350	T351	G352	K353	Y354	A355	R356	N357	A360	H361	T362	M363	D364	V365	K366	Q367	L368	T369	E370	A371	V372	Q373	K374	I375	T376	T377	
I257	Q258	K259	L260	V261	G262	K263	L264	N265	W266	A267	S268	Q269	I270	Y271	P272	G273	I274	W275	V276	R277	Q278	L279	S280	K281	L282	L283	R284	G285	T286	K287	A288	L289	T290	E291	V292	L293	P294	L295	T296	E297	E298	A299	E300	L301	E302	L303	A304	E305	N306	R307	E308	I309	L310	K311	E312	P313	V314	G316
I195	G196	Q197	H198	R199	T200	K201	L202	E203	E204	L205	R206	Q207	H208	L209	L210	L211	W212	G213	L214	T215	T216	D218	K219	A158	K220	H221	Q222	Q223	E224	P225	P226	W229	Y232	E233	L234	H235	P236	D237	K238	W239	T240	V241	Q242	P243	I244	V245	L246	P247	E248	K249	D250	S251	W252	T253	V254	N255	D256	
I131	I132	P133	S134	I135	M136	T140	R143	Y144	Q145	Y146	M147	V148	L149	L150	Q151	G152	W153	K154	G155	P157	S156	P157	A158	I159	F160	Q161	S162	S163	M164	T165	K166	I167	L168	E169	P170	F171	K172	K173	Q174	M175	P176	D177	I178	V179	I180	Y181	Q182	Y183	W184	L187	Y188	Y189	G190	S191	D192	A193	E194	
I63	K64	K65	K66	D67	S68	T69	K70	W71	R72	K73	L74	W75	D76	F77	L80	N81	W82	R83	Q85	D86	F87	H88	E89	V90	Q91	L92	G93	I94	F95	H96	P97	K103	T107	V108	L109	D110	V111	G112	D113	A114	Y115	F116	S117	L120	D121	E122	D123	F124	R125	K126	Y127	T128	A129	F130				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.00Å 69.30Å 104.10Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 82.5 (19.95-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.88Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.259 , (Not available) 0.269 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 200.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 28378 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7845	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TB9

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	0.71	1/4497 (0.0%)	0.98	10/6132 (0.2%)
2	B	0.77	3/3541 (0.1%)	0.99	7/4822 (0.1%)
All	All	0.74	4/8038 (0.0%)	0.98	17/10954 (0.2%)

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
2	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	CYS	CB-SG	-5.32	1.73	1.81
1	A	337	TRP	CB-CG	-5.25	1.40	1.50
2	B	153	TRP	CB-CG	-5.21	1.40	1.50
2	B	266	TRP	CB-CG	5.09	1.59	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	325	LEU	CA-CB-CG	7.62	132.82	115.30
2	B	244	ILE	N-CA-C	-6.38	93.76	111.00
1	A	420	PRO	C-N-CD	6.19	141.40	128.40
1	A	420	PRO	N-CA-C	6.17	128.14	112.10
2	B	226	PRO	N-CA-CB	6.14	110.66	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	427	TYR	Sidechain

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	4382	0	4279	576	0
2	B	3442	0	3405	410	0
3	A	21	0	20	15	0
All	All	7845	0	7704	962	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 62.

The worst 5 of 962 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:60:VAL:HA	1:A:75:VAL:HG22	1.24	1.17
1:A:420:PRO:HG2	1:A:421:PRO:HD3	1.31	1.10
1:A:419:THR:HG22	1:A:420:PRO:HD3	1.09	1.09
2:B:282:LEU:HG	2:B:293:ILE:HG22	1.32	1.09
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.36	1.07

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	556/558 (100%)	381 (68%)	129 (23%)	46 (8%)	1	5
2	B	425/427 (100%)	291 (68%)	88 (21%)	46 (11%)	0	2
All	All	981/985 (100%)	672 (68%)	217 (22%)	92 (9%)	1	4

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	213	GLY
1	A	412	PRO
1	A	462	GLY
1	A	474	ASN

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	457/498 (92%)	372 (81%)	85 (19%)	2	10
2	B	367/389 (94%)	305 (83%)	62 (17%)	2	13
All	All	824/887 (93%)	677 (82%)	147 (18%)	2	11

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	THR
1	A	540	LYS
2	B	340	GLN
1	A	497	THR
1	A	513	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	54	ASN

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Mol	Chain	Res	Type
2	B	57	ASN
2	B	255	ASN
1	A	487	GLN
2	B	207	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	TB9	A	600	-	19,23,23	2.77	7 (36%)	16,34,34	2.86	5 (31%)

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
3	TB9	A	600	-	-	0/4/17/17	0/2/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	TB9	C4-N3	-4.08	1.45	1.49
3	A	600	TB9	C12-C13	-3.26	1.46	1.50
3	A	600	TB9	C10-C1A	-2.22	1.38	1.41
3	A	600	TB9	C10-C9	3.44	1.43	1.36
3	A	600	TB9	C8-C7A	4.93	1.45	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	TB9	C15-C14-C13	-4.66	107.63	122.61
3	A	600	TB9	C8-C7A-C3A	-3.02	115.44	118.44
3	A	600	TB9	C13-C12-N6	-2.83	106.02	112.53
3	A	600	TB9	C2-N1-C1A	2.44	108.66	103.66
3	A	600	TB9	C16-C14-C15	8.42	135.34	114.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	TB9	15	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	558/558 (100%)	0.04	11 (1%) 68 39	10, 45, 64, 65	0
2	B	427/427 (100%)	-0.02	17 (3%) 42 17	10, 34, 65, 65	0
All	All	985/985 (100%)	0.01	28 (2%) 56 27	10, 43, 65, 65	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	SER	5.6
1	A	552	VAL	4.6
2	B	222	GLN	4.4
2	B	197	GLN	4.3
2	B	2	ILE	3.4

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
3	TB9	A	600	21/21	0.85	0.26	0.23	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.