



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:24 PM UTC

PDB ID : 2F37 / pdb_00002f37
Title : Crystal structure of the ankyrin repeat domain of human TRPV2
Authors : McCleverty, C.J.
Deposited on : 2005-11-18
Resolution : 1.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

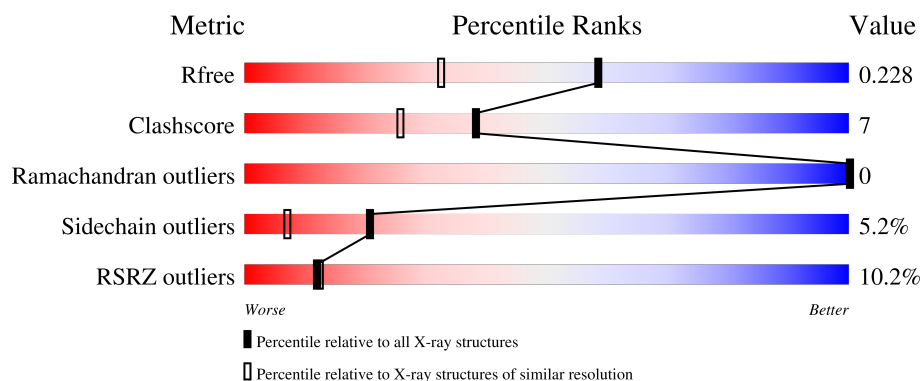
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	251	
1	B	251	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4287 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.

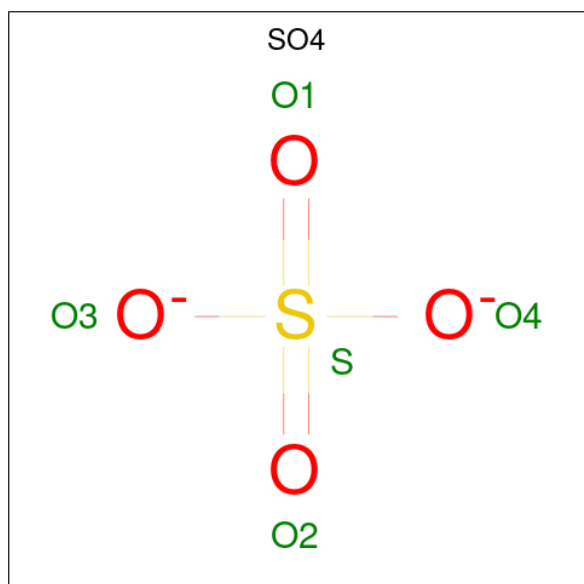
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	Se	17	5	0
			1936	1216	340	368	9	3			
1	B	249	Total	C	N	O	S	Se	5	5	0
			1952	1225	342	374	8	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MSE	MET	modified residue	UNP Q9Y5S1
A	254	MSE	MET	modified residue	UNP Q9Y5S1
A	269	MSE	MET	modified residue	UNP Q9Y5S1
B	121	MSE	MET	modified residue	UNP Q9Y5S1
B	254	MSE	MET	modified residue	UNP Q9Y5S1
B	269	MSE	MET	modified residue	UNP Q9Y5S1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

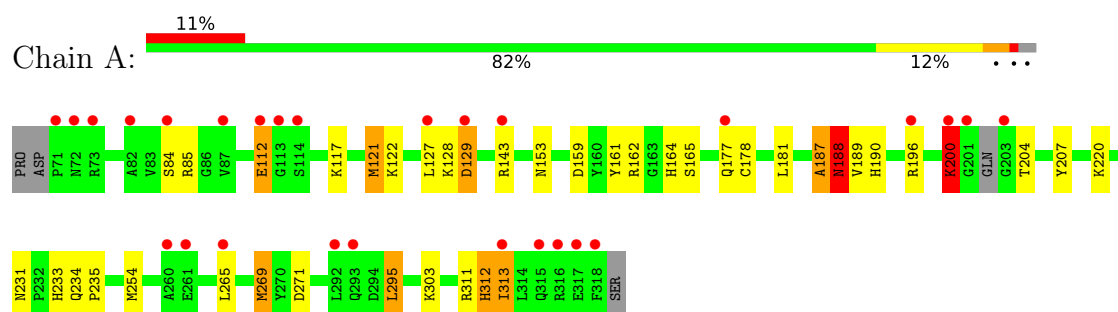
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total	O	0	0
			199	199		
3	B	190	Total	O	0	0
			190	190		

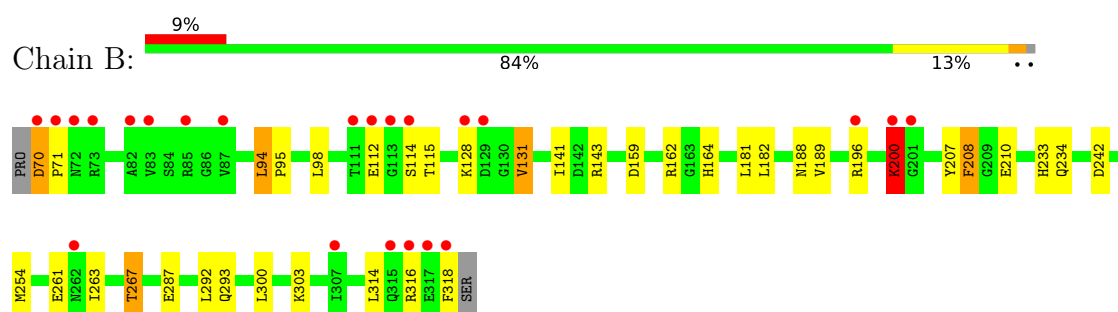
3 Residue-property plots

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: Transient receptor potential cation channel subfamily V member 2



- Molecule 1: Transient receptor potential cation channel subfamily V member 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.66Å 93.66Å 265.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.70) 99.8 (50.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.229 (Not available) , 0.228	Depositor DCC
R_{free} test set	4150 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.6	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	0.95	EDS
Total number of atoms	4287	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.58	1/1981 (0.1%)	1.02	5/2676 (0.2%)
1	B	0.60	0/1998	0.83	4/2701 (0.1%)
All	All	0.59	1/3979 (0.0%)	0.93	9/5377 (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
1	A	0	3
1	B	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	MSE	SE-CE	-5.52	1.78	1.95

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ILE	N-CA-C	-31.42	86.45	111.90
1	A	188	ASN	N-CA-C	-10.39	90.43	108.20
1	B	208	PHE	N-CA-C	10.11	126.13	111.87
1	B	208	PHE	N-CA-CB	-7.45	99.77	111.39
1	A	269	MSE	CB-CG-SE	-6.73	92.52	112.70
1	A	129	ASP	N-CA-C	-5.76	105.55	112.58
1	A	269	MSE	N-CA-CB	5.36	118.09	110.16
1	B	131	VAL	N-CA-C	5.20	116.21	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	THR	N-CA-C	-5.11	107.72	114.31

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ALA	Peptide
1	A	200	LYS	Peptide
1	A	312	HIS	Peptide
1	B	112	GLU	Peptide
1	B	200	LYS	Peptide
1	B	207	TYR	Peptide

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	1936	0	1946	31	0
1	B	1952	0	1952	23	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	199	0	0	6	1
3	B	190	0	0	4	1
All	All	4287	0	3898	53	1

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 (53) 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:231:ASN:HD21	1:A:234:GLN:H	1.29	0.76
1:A:143:ARG:HD3	3:A:652:HOH:O	1.88	0.73
1:A:231:ASN:HD22	1:A:233:HIS:H	1.39	0.70
1:A:271:ASP:OD1	1:A:312:HIS:HE1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ASP:N	1:B:71:PRO:HD2	2.09	0.68
1:A:177:GLN:HG2	3:A:503:HOH:O	1.92	0.68
1:B:200:LYS:HD3	1:B:254:MSE:HE3	1.75	0.66
1:B:188:ASN:HA	1:B:234:GLN:HE22	1.64	0.62
1:A:159:ASP:HB3	1:A:196:ARG:NH1	2.15	0.61
1:B:316:ARG:HG3	3:B:558:HOH:O	2.03	0.59
1:A:128:LYS:O	1:A:129:ASP:HB2	2.02	0.58
1:A:127:LEU:HD21	1:A:178[B]:CYS:SG	2.45	0.57
1:A:200:LYS:HE3	1:A:254:MSE:HE2	1.86	0.57
1:A:189:VAL:H	1:A:234:GLN:NE2	2.01	0.56
1:B:263:ILE:O	1:B:267:THR:HB	2.05	0.56
1:B:159:ASP:HB3	1:B:196:ARG:NH2	2.21	0.56
1:A:295:LEU:HD21	1:A:303:LYS:HD2	1.89	0.54
1:A:153:ASN:HD21	1:A:187:ALA:HA	1.73	0.54
1:A:200:LYS:CE	1:A:254:MSE:HE2	2.38	0.53
1:B:189:VAL:H	1:B:234:GLN:NE2	2.06	0.52
1:A:159:ASP:CB	1:A:196:ARG:NH1	2.72	0.52
1:B:164:HIS:HE1	3:B:513:HOH:O	1.91	0.52
1:A:164:HIS:HE1	3:A:531:HOH:O	1.93	0.51
1:A:235:PRO:HD2	1:B:143:ARG:HD2	1.94	0.50
1:A:188:ASN:ND2	1:A:190:HIS:H	2.09	0.50
1:A:220:LYS:HG3	1:A:265:LEU:HD23	1.94	0.50
1:B:159:ASP:HB3	1:B:196:ARG:HH22	1.77	0.50
1:B:70:ASP:OD2	1:B:71:PRO:HD3	2.12	0.49
1:B:316:ARG:C	1:B:318:PHE:H	2.21	0.48
1:A:231:ASN:ND2	1:A:233:HIS:H	2.07	0.48
1:B:70:ASP:N	1:B:71:PRO:CD	2.77	0.48
1:A:164:HIS:HD2	3:A:644:HOH:O	1.96	0.47
1:B:208:PHE:CD1	1:B:208:PHE:N	2.81	0.46
1:B:95:PRO:HG3	1:B:141:ILE:HG12	1.97	0.46
1:A:200:LYS:HD2	1:A:207:TYR:CE1	2.51	0.45
1:A:84:SER:OG	1:A:122:LYS:HE3	2.16	0.45
1:A:121:MSE:HE2	1:A:165:SER:HA	1.99	0.45
1:B:159:ASP:OD1	1:B:162:ARG:NH1	2.48	0.44
1:A:188:ASN:C	1:A:188:ASN:HD22	2.27	0.43
1:B:287:GLU:CD	1:B:316:ARG:HH12	2.27	0.43
1:A:153:ASN:HD21	1:A:188:ASN:N	2.16	0.43
1:B:94:LEU:HD22	1:B:98:LEU:HG	2.01	0.42
1:B:303:LYS:NZ	3:B:640:HOH:O	2.52	0.42
1:A:112:GLU:HB2	1:A:117:LYS:HB3	2.02	0.42
1:B:94:LEU:HB3	1:B:95:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:O	1:A:162:ARG:C	2.63	0.42
3:A:554:HOH:O	1:B:233:HIS:HD2	2.03	0.42
1:A:312:HIS:HD2	3:A:633:HOH:O	2.02	0.42
1:A:189:VAL:H	1:A:234:GLN:HE22	1.68	0.41
1:B:293:GLN:HG2	3:B:640:HOH:O	2.20	0.41
1:A:188:ASN:HA	1:A:234:GLN:HE22	1.86	0.41
1:A:311:ARG:O	1:A:312:HIS:C	2.63	0.41
1:B:210:GLU:CD	1:B:242:ASP:HB2	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:679:HOH:O	3:B:626:HOH:O[8_566]	0.33	1.87

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	248/251 (99%)	243 (98%)	5 (2%)	0	100	100
1	B	252/251 (100%)	244 (97%)	8 (3%)	0	100	100
All	All	500/502 (100%)	487 (97%)	13 (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	215/211 (102%)	206 (96%)	9 (4%)	26	11
1	B	217/211 (103%)	204 (94%)	13 (6%)	17	5
All	All	432/422 (102%)	410 (95%)	22 (5%)	21	7

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	112	GLU
1	A	181	LEU
1	A	188	ASN
1	A	200	LYS
1	A	204	THR
1	A	269	MSE
1	A	295	LEU
1	A	313	ILE
1	B	70	ASP
1	B	94	LEU
1	B	114	SER
1	B	128	LYS
1	B	131	VAL
1	B	181	LEU
1	B	182	LEU
1	B	200	LYS
1	B	261	GLU
1	B	267	THR
1	B	292	LEU
1	B	300	LEU
1	B	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	164	HIS
1	A	177	GLN
1	A	188	ASN
1	A	231	ASN

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	244	GLN
1	A	258	ASN
1	A	262	ASN
1	A	312	HIS
1	A	315	GLN
1	B	140	GLN
1	B	155	GLN
1	B	164	HIS
1	B	233	HIS
1	B	234	GLN
1	B	239	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](#)

2 ligands are 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	$\# Z > 2$
2	SO4	B	501	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	244/251 (97%)	0.55	27 (11%)	10 10	11, 22, 35, 50	11 (4%)
1	B	246/251 (98%)	0.53	23 (9%)	14 15	10, 21, 38, 48	6 (2%)
All	All	490/502 (97%)	0.54	50 (10%)	12 12	10, 22, 37, 50	17 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	PRO	16.8
1	B	113	GLY	5.4
1	B	200	LYS	5.0
1	B	70	ASP	4.7
1	A	318	PHE	4.7
1	B	316	ARG	4.5
1	B	318	PHE	4.5
1	A	82	ALA	4.1
1	B	128	LYS	4.1
1	B	71	PRO	4.0
1	B	114	SER	4.0
1	A	316	ARG	3.9
1	A	313	ILE	3.6
1	B	72	ASN	3.6
1	B	83	VAL	3.5
1	B	82	ALA	3.4
1	A	317	GLU	3.4
1	A	261	GLU	3.2
1	A	201	GLY	3.1
1	A	73	ARG	3.0
1	A	87	VAL	3.0
1	A	265	LEU	3.0
1	B	315	GLN	2.9
1	A	112	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	85	ARG	2.9
1	B	112	GLU	2.7
1	B	87	VAL	2.7
1	B	201	GLY	2.6
1	A	129	ASP	2.6
1	B	307	ILE	2.6
1	B	317	GLU	2.5
1	A	203	GLY	2.5
1	A	114	SER	2.5
1	A	260	ALA	2.4
1	B	262	ASN	2.4
1	B	196	ARG	2.4
1	A	196	ARG	2.4
1	A	143	ARG	2.3
1	B	129	ASP	2.3
1	A	315	GLN	2.3
1	A	200	LYS	2.3
1	B	73	ARG	2.2
1	A	127	LEU	2.2
1	A	72	ASN	2.2
1	A	293	GLN	2.2
1	A	84	SER	2.2
1	A	177	GLN	2.1
1	B	111	THR	2.1
1	A	113	GLY	2.1
1	A	292	LEU	2.1

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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	502	5/5	0.86	0.13	71,71,71,71	0
2	SO4	B	501	5/5	0.95	0.08	34,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.