



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:15 AM EDT

PDB ID : 9LBF / pdb_00009lbf
Title : The crystal structure of the truncated PAK2 containing D368N mutant
Authors : Hu, H.-F.; Luo, Z.P.; Wu, J.-W.; Wang, Z.-X.
Deposited on : 2025-01-03
Resolution : 2.62 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

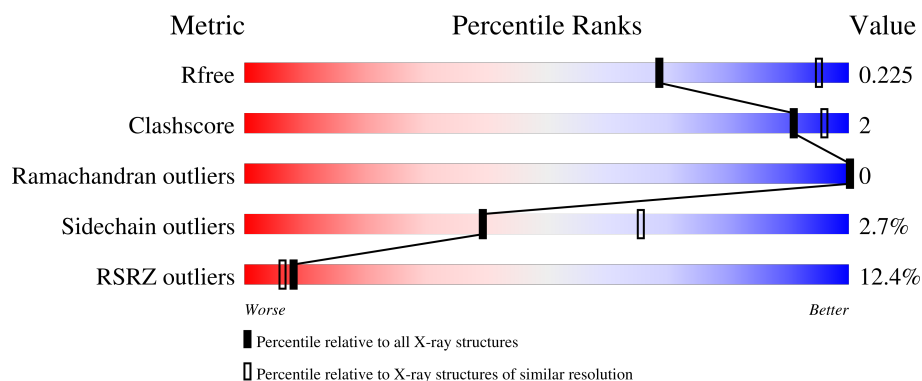
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	479	8% 67% 5% 27%
1	B	479	10% 63% 5% 32%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5474 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 Serine/threonine-protein kinase PAK 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2757	1767	452	520	18			
1	B	324	Total	C	N	O	S	0	0	0
			2533	1619	416	480	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MET	-	initiating methionine	UNP Q13177
A	47	GLY	-	expression tag	UNP Q13177
A	48	SER	-	expression tag	UNP Q13177
A	49	SER	-	expression tag	UNP Q13177
A	50	HIS	-	expression tag	UNP Q13177
A	51	HIS	-	expression tag	UNP Q13177
A	52	HIS	-	expression tag	UNP Q13177
A	53	HIS	-	expression tag	UNP Q13177
A	54	HIS	-	expression tag	UNP Q13177
A	55	HIS	-	expression tag	UNP Q13177
A	56	SER	-	expression tag	UNP Q13177
A	57	SER	-	expression tag	UNP Q13177
A	58	GLY	-	expression tag	UNP Q13177
A	59	LEU	-	expression tag	UNP Q13177
A	60	VAL	-	expression tag	UNP Q13177
A	61	PRO	-	expression tag	UNP Q13177
A	62	ARG	-	expression tag	UNP Q13177
A	63	GLY	-	expression tag	UNP Q13177
A	64	SER	-	expression tag	UNP Q13177
A	65	HIS	-	expression tag	UNP Q13177
A	66	MET	-	expression tag	UNP Q13177
A	67	ALA	-	expression tag	UNP Q13177
A	68	SER	-	expression tag	UNP Q13177
A	368	ASN	ASP	engineered mutation	UNP Q13177
B	46	MET	-	initiating methionine	UNP Q13177

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Chain	Residue	Modelled	Actual	Comment	Reference
B	47	GLY	-	expression tag	UNP Q13177
B	48	SER	-	expression tag	UNP Q13177
B	49	SER	-	expression tag	UNP Q13177
B	50	HIS	-	expression tag	UNP Q13177
B	51	HIS	-	expression tag	UNP Q13177
B	52	HIS	-	expression tag	UNP Q13177
B	53	HIS	-	expression tag	UNP Q13177
B	54	HIS	-	expression tag	UNP Q13177
B	55	HIS	-	expression tag	UNP Q13177
B	56	SER	-	expression tag	UNP Q13177
B	57	SER	-	expression tag	UNP Q13177
B	58	GLY	-	expression tag	UNP Q13177
B	59	LEU	-	expression tag	UNP Q13177
B	60	VAL	-	expression tag	UNP Q13177
B	61	PRO	-	expression tag	UNP Q13177
B	62	ARG	-	expression tag	UNP Q13177
B	63	GLY	-	expression tag	UNP Q13177
B	64	SER	-	expression tag	UNP Q13177
B	65	HIS	-	expression tag	UNP Q13177
B	66	MET	-	expression tag	UNP Q13177
B	67	ALA	-	expression tag	UNP Q13177
B	68	SER	-	expression tag	UNP Q13177
B	368	ASN	ASP	engineered mutation	UNP Q13177

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

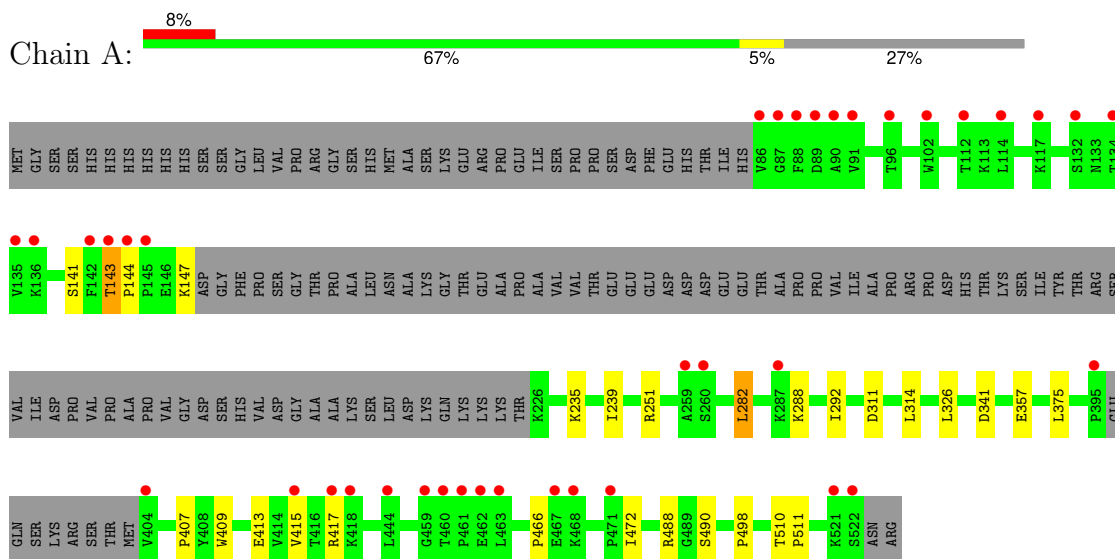
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	83	Total	O	0	0
			83	83		

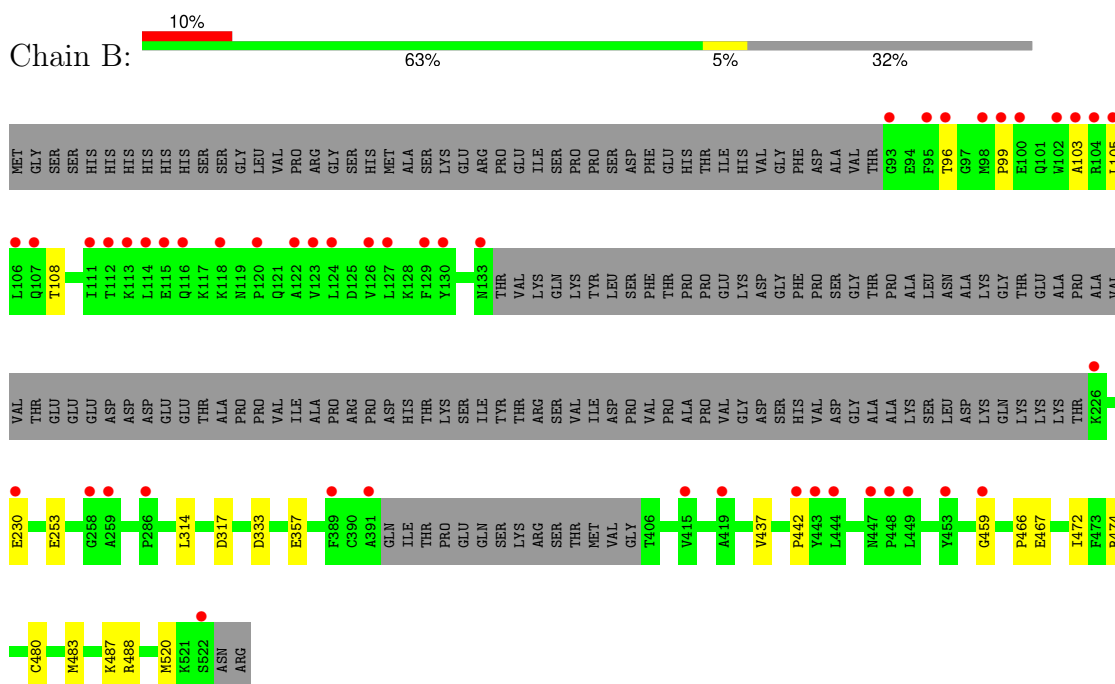
3 Residue-property plots [i](#)

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: Serine/threonine-protein kinase PAK 2



- Molecule 1: Serine/threonine-protein kinase PAK 2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	167.32Å 167.32Å 212.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.89 – 2.62 42.89 – 2.62	Depositor EDS
% Data completeness (in resolution range)	89.1 (42.89-2.62) 89.3 (42.89-2.62)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.198 , 0.222 0.204 , 0.225	Depositor DCC
R_{free} test set	1471 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.017 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.005 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5474	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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	0.65	0/2806	1.09	2/3794 (0.1%)
1	B	0.64	0/2576	1.09	3/3481 (0.1%)
All	All	0.65	0/5382	1.09	5/7275 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	PRO	N-CA-C	5.70	121.33	113.98
1	A	341	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	230	GLU	CB-CG-CD	5.55	122.04	112.60
1	B	442	PRO	N-CA-C	5.20	120.43	114.03
1	B	317	ASP	CA-CB-CG	5.10	117.70	112.60

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	2757	0	2824	9	0
1	B	2533	0	2574	10	0
2	A	15	0	0	0	0
2	B	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	66	0	0	0	0
3	B	83	0	0	0	0
All	All	5474	0	5398	18	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 2.

All (18) 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:472:ILE:HD11	1:A:498:PRO:HG2	1.82	0.60
1:B:99:PRO:CG	1:B:103:ALA:HB2	2.34	0.58
1:A:282:LEU:O	1:A:288:LYS:HE3	2.07	0.54
1:B:466:PRO:HA	2:B:603:SO4:O2	2.08	0.54
1:A:413:GLU:CD	1:A:488:ARG:HH12	2.15	0.53
1:A:143:THR:N	1:A:144:PRO:CD	2.76	0.49
1:B:105:LEU:HA	1:B:108:THR:HG22	1.96	0.48
1:B:459:GLY:HA2	1:B:483:MET:SD	2.56	0.46
1:A:326:LEU:HB2	1:A:375:LEU:HG	1.97	0.46
1:B:467:GLU:O	1:B:474:ARG:NH1	2.48	0.45
1:A:251:ARG:NE	1:B:253:GLU:OE1	2.49	0.45
1:A:510:THR:N	1:A:511:PRO:HD2	2.33	0.43
1:A:407:PRO:HA	1:A:409:TRP:CZ3	2.54	0.43
1:B:480:CYS:O	1:B:488:ARG:HD2	2.18	0.43
1:B:99:PRO:HG2	1:B:103:ALA:HB2	2.00	0.42
1:B:333:ASP:HA	1:B:520:MET:HE3	2.02	0.42
1:B:472:ILE:HD12	1:B:472:ILE:HA	1.97	0.41
1:A:235:LYS:HB3	1:A:292:ILE:HG21	2.02	0.41

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	345/479 (72%)	335 (97%)	10 (3%)	0	100	100
1	B	318/479 (66%)	309 (97%)	9 (3%)	0	100	100
All	All	663/958 (69%)	644 (97%)	19 (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	307/417 (74%)	296 (96%)	11 (4%)	31	56
1	B	279/417 (67%)	274 (98%)	5 (2%)	51	75
All	All	586/834 (70%)	570 (97%)	16 (3%)	39	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	A	143	THR
1	A	147	LYS
1	A	239	ILE
1	A	282	LEU
1	A	311	ASP
1	A	314	LEU
1	A	357	GLU
1	A	415	VAL
1	A	417	ARG
1	A	490	SER
1	B	96	THR
1	B	314	LEU
1	B	357	GLU
1	B	437	VAL
1	B	487	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	GLN
1	A	305	ASN
1	A	392	GLN
1	B	101	GLN
1	B	116	GLN
1	B	133	ASN
1	B	273	GLN
1	B	279	GLN
1	B	285	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](#)

7 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	A	601	-	4,4,4	0.45	0	6,6,6	0.39	0
2	SO4	A	603	-	4,4,4	0.45	0	6,6,6	0.20	0
2	SO4	B	604	-	4,4,4	0.21	0	6,6,6	0.20	0
2	SO4	B	601	-	4,4,4	0.32	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	602	-	4,4,4	0.32	0	6,6,6	0.16	0
2	SO4	B	602	-	4,4,4	0.34	0	6,6,6	0.18	0
2	SO4	B	603	-	4,4,4	0.32	0	6,6,6	0.22	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	SO4	1	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 ⓘ

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	351/479 (73%)	0.47	38 (10%) 11 8	18, 49, 111, 175	0
1	B	324/479 (67%)	0.47	46 (14%) 6 5	16, 46, 134, 184	0
All	All	675/958 (70%)	0.47	84 (12%) 8 6	16, 47, 127, 184	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	VAL	6.0
1	A	144	PRO	6.0
1	A	521	LYS	5.9
1	A	404	VAL	5.7
1	B	259	ALA	5.2
1	A	522	SER	5.1
1	A	86	VAL	5.1
1	A	460	THR	5.1
1	A	142	PHE	5.0
1	A	461	PRO	5.0
1	A	135	VAL	4.8
1	A	143	THR	4.6
1	A	145	PRO	4.5
1	B	124	LEU	4.5
1	A	114	LEU	4.4
1	B	106	LEU	4.4
1	B	102	TRP	4.2
1	B	103	ALA	4.2
1	A	260	SER	4.1
1	B	114	LEU	4.1
1	B	444	LEU	4.1
1	A	418	LYS	4.0
1	B	112	THR	4.0
1	A	117	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	462	GLU	3.7
1	B	107	GLN	3.7
1	B	443	TYR	3.6
1	A	395	PRO	3.5
1	B	459	GLY	3.5
1	B	449	LEU	3.5
1	A	463	LEU	3.5
1	B	122	ALA	3.4
1	B	104	ARG	3.3
1	A	102	TRP	3.2
1	B	391	ALA	3.1
1	B	111	ILE	3.0
1	A	90	ALA	2.9
1	B	113	LYS	2.9
1	B	105	LEU	2.8
1	A	467	GLU	2.8
1	A	259	ALA	2.8
1	B	95	PHE	2.8
1	B	453	TYR	2.7
1	B	96	THR	2.7
1	B	118	LYS	2.7
1	B	93	GLY	2.7
1	B	127	LEU	2.6
1	B	448	PRO	2.6
1	A	136	LYS	2.6
1	A	468	LYS	2.5
1	A	417	ARG	2.5
1	A	132	SER	2.5
1	A	471	PRO	2.5
1	B	415	VAL	2.5
1	A	287	LYS	2.4
1	B	442	PRO	2.4
1	B	389	PHE	2.4
1	B	116	GLN	2.4
1	B	522	SER	2.3
1	B	123	VAL	2.3
1	A	444	LEU	2.3
1	B	130	TYR	2.2
1	A	89	ASP	2.2
1	A	112	THR	2.2
1	B	133	ASN	2.2
1	B	447	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	126	VAL	2.2
1	A	88	PHE	2.2
1	B	230	GLU	2.2
1	A	459	GLY	2.2
1	B	258	GLY	2.2
1	B	419	ALA	2.1
1	A	96	THR	2.1
1	B	286	PRO	2.1
1	B	226	LYS	2.1
1	A	87	GLY	2.1
1	B	129	PHE	2.1
1	B	120	PRO	2.1
1	B	98	MET	2.1
1	B	99	PRO	2.1
1	B	100	GLU	2.0
1	B	115	GLU	2.0
1	A	415	VAL	2.0
1	A	134	THR	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](#)

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(Å ²)	Q<0.9
2	SO4	B	604	5/5	0.77	0.15	73,81,109,115	0
2	SO4	B	603	5/5	0.79	0.14	86,88,107,124	0
2	SO4	B	601	5/5	0.93	0.13	66,68,72,73	5
2	SO4	A	603	5/5	0.94	0.12	44,45,53,76	5
2	SO4	A	602	5/5	0.94	0.11	57,58,64,72	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	601	5/5	0.95	0.12	45,48,56,56	5
2	SO4	B	602	5/5	0.98	0.07	40,45,56,62	5

6.5 Other polymers [i](#)

There are no such residues in this entry.