



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2026 – 11:25 PM JST

PDB ID : 9WS5 / pdb_00009ws5
Title : Crystal structure of PAK2 kinase domain containing D368N mutant
Authors : Chen, F.Y.; Hu, H.-F.; Wang, J.; Luo, Z.P.; Wu, J.-W.; Wang, Z.-X.
Deposited on : 2025-09-12
Resolution : 2.40 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

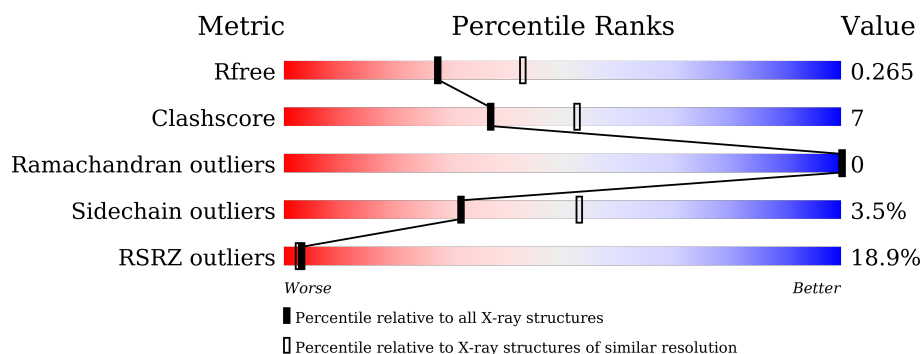
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	323	16% 70% 13% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2115 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.

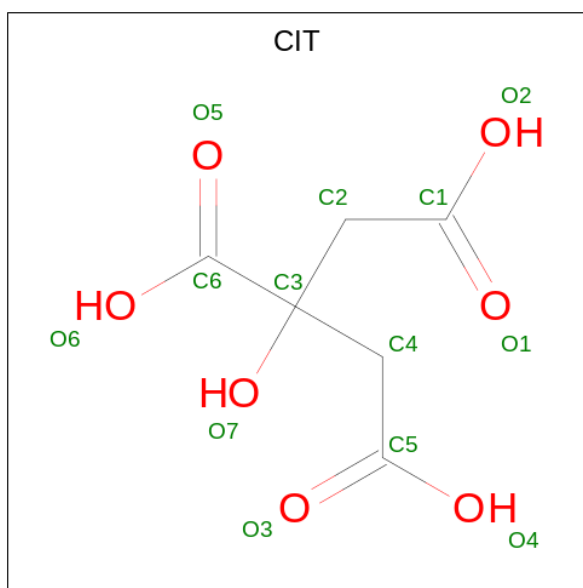
- Molecule 1 is a protein called PAK-2p34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2084	1326	345	398	15			

There are 27 discrepancies between the modelled and reference sequences:

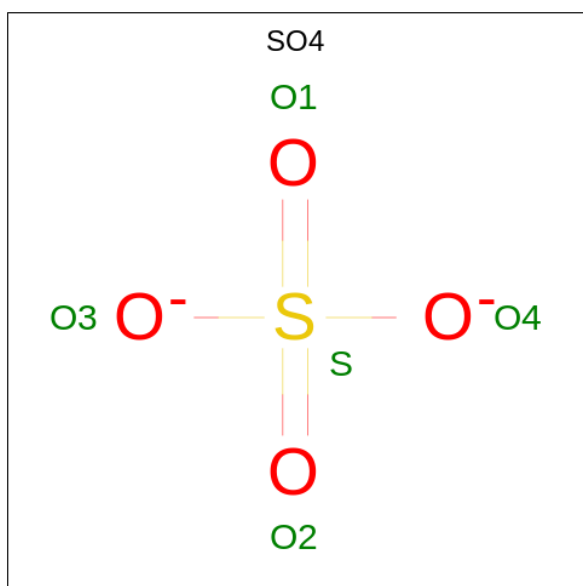
Chain	Residue	Modelled	Actual	Comment	Reference
A	202	MET	-	initiating methionine	UNP Q13177
A	203	GLY	-	expression tag	UNP Q13177
A	204	SER	-	expression tag	UNP Q13177
A	205	SER	-	expression tag	UNP Q13177
A	206	HIS	-	expression tag	UNP Q13177
A	207	HIS	-	expression tag	UNP Q13177
A	208	HIS	-	expression tag	UNP Q13177
A	209	HIS	-	expression tag	UNP Q13177
A	210	HIS	-	expression tag	UNP Q13177
A	211	HIS	-	expression tag	UNP Q13177
A	212	SER	-	expression tag	UNP Q13177
A	213	GLN	-	expression tag	UNP Q13177
A	214	ASP	-	expression tag	UNP Q13177
A	215	LEU	-	expression tag	UNP Q13177
A	216	GLU	-	expression tag	UNP Q13177
A	217	VAL	-	expression tag	UNP Q13177
A	218	LEU	-	expression tag	UNP Q13177
A	219	PHE	-	expression tag	UNP Q13177
A	220	GLN	-	expression tag	UNP Q13177
A	221	GLY	-	expression tag	UNP Q13177
A	222	PRO	-	expression tag	UNP Q13177
A	223	HIS	-	expression tag	UNP Q13177
A	224	MET	-	expression tag	UNP Q13177
A	225	ALA	-	expression tag	UNP Q13177
A	226	ASP	-	expression tag	UNP Q13177
A	227	LEU	-	expression tag	UNP Q13177
A	368	ASN	ASP	engineered mutation	UNP Q13177

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

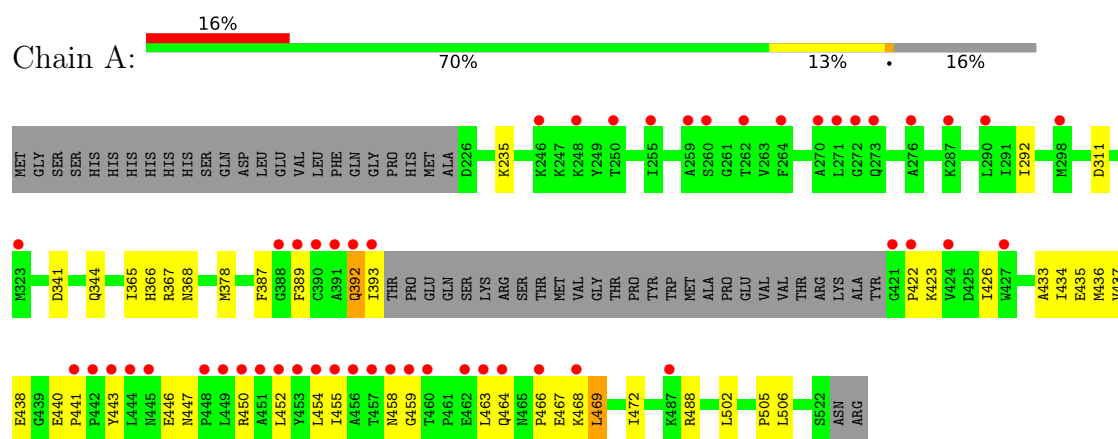


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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: PAK-2p34



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.53Å 97.53Å 144.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.22 – 2.40 46.22 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.22-2.40) 99.9 (46.22-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.242 , 0.263 0.245 , 0.265	Depositor DCC
R_{free} test set	803 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2115	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, 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	0.60	0/2114	1.09	0/2854

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2084	0	2122	30	0
2	A	26	0	10	4	0
3	A	5	0	0	0	0
All	All	2115	0	2132	30	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 7.

All (30) 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:438:GLU:HG3	1:A:440:GLU:HG2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ILE:HG12	1:A:463:LEU:HD21	1.69	0.73
1:A:443:TYR:O	1:A:447:ASN:N	2.32	0.61
1:A:392:GLN:O	1:A:393:ILE:C	2.42	0.61
1:A:463:LEU:O	1:A:466:PRO:HD2	2.01	0.59
1:A:423:LYS:O	1:A:488:ARG:NH1	2.35	0.58
1:A:447:ASN:HB3	1:A:450:ARG:HB2	1.86	0.57
1:A:455:ILE:C	1:A:458:ASN:H	2.16	0.54
1:A:454:LEU:O	1:A:459:GLY:N	2.42	0.50
1:A:437:VAL:HG11	1:A:469:LEU:HD21	1.94	0.49
1:A:472:ILE:HD11	1:A:502:LEU:HD11	1.95	0.48
1:A:441:PRO:HG2	1:A:446:GLU:HG3	1.96	0.47
1:A:389:PHE:HD2	1:A:392:GLN:HE22	1.62	0.47
1:A:455:ILE:O	1:A:458:ASN:N	2.49	0.46
1:A:341:ASP:OD1	1:A:344:GLN:HG3	2.16	0.45
1:A:378:MET:N	2:A:601:CIT:O7	2.48	0.45
1:A:463:LEU:HD22	1:A:469:LEU:HD11	1.97	0.45
1:A:366:HIS:CE1	1:A:368:ASN:HB2	2.52	0.45
1:A:423:LYS:HA	1:A:426:ILE:HG12	1.99	0.44
1:A:422:PRO:O	1:A:423:LYS:HB2	2.18	0.44
1:A:506:LEU:H	2:A:602:CIT:HO7	1.62	0.44
1:A:506:LEU:N	2:A:602:CIT:O7	2.39	0.43
1:A:505:PRO:HA	2:A:602:CIT:C5	2.49	0.42
1:A:438:GLU:CG	1:A:440:GLU:HG2	2.41	0.42
1:A:365:ILE:HG22	1:A:367:ARG:HG3	2.02	0.42
1:A:433:ALA:O	1:A:437:VAL:HG23	2.20	0.41
1:A:235:LYS:HB3	1:A:292:ILE:HG21	2.01	0.41
1:A:433:ALA:HA	1:A:436:MET:HE3	2.01	0.41
1:A:435:GLU:HG3	1:A:440:GLU:O	2.21	0.40
1:A:463:LEU:C	1:A:466:PRO:HD2	2.46	0.40

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	266/323 (82%)	256 (96%)	10 (4%)	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	229/282 (81%)	221 (96%)	8 (4%)	32	53

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	ASP
1	A	387	PHE
1	A	392	GLN
1	A	452	LEU
1	A	464	GLN
1	A	467	GLU
1	A	468	LYS
1	A	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	354	GLN
1	A	464	GLN
1	A	465	ASN

5.3.3 RNA ⓘ

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](#)

3 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	CIT	A	602	-	12,12,12	1.27	0	17,17,17	1.68	4 (23%)
2	CIT	A	601	-	12,12,12	1.32	2 (16%)	17,17,17	1.41	3 (17%)
3	SO4	A	603	-	4,4,4	0.48	0	6,6,6	0.95	0

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
2	CIT	A	602	-	-	7/16/16/16	-
2	CIT	A	601	-	-	7/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	CIT	O2-C1	-2.83	1.21	1.30
2	A	601	CIT	C3-C6	2.27	1.55	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	CIT	O5-C6-C3	-4.20	116.31	122.25
2	A	601	CIT	O5-C6-C3	-3.68	117.04	122.25
2	A	602	CIT	O6-C6-C3	3.04	118.32	113.05
2	A	601	CIT	O6-C6-C3	2.82	117.95	113.05
2	A	602	CIT	C3-C2-C1	2.22	119.18	113.81
2	A	602	CIT	C3-C4-C5	2.21	119.17	113.81
2	A	601	CIT	O3-C5-C4	-2.09	116.84	122.94

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CIT	C2-C3-C4-C5
2	A	601	CIT	O7-C3-C4-C5
2	A	601	CIT	C6-C3-C4-C5
2	A	601	CIT	C2-C3-C6-O5
2	A	601	CIT	C2-C3-C6-O6
2	A	601	CIT	O7-C3-C6-O5
2	A	601	CIT	O7-C3-C6-O6
2	A	602	CIT	C1-C2-C3-O7
2	A	602	CIT	C1-C2-C3-C4
2	A	602	CIT	C1-C2-C3-C6
2	A	602	CIT	C2-C3-C6-O5
2	A	602	CIT	C2-C3-C6-O6
2	A	602	CIT	O7-C3-C6-O5
2	A	602	CIT	O7-C3-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	CIT	3	0
2	A	601	CIT	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	270/323 (83%)	1.00	51 (18%) 3 2	31, 72, 156, 190	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	TYR	6.0
1	A	393	ILE	5.9
1	A	463	LEU	5.9
1	A	452	LEU	5.4
1	A	444	LEU	5.3
1	A	451	ALA	5.0
1	A	391	ALA	4.9
1	A	459	GLY	4.8
1	A	458	ASN	4.4
1	A	454	LEU	4.4
1	A	455	ILE	4.0
1	A	271	LEU	3.8
1	A	449	LEU	3.8
1	A	456	ALA	3.7
1	A	453	TYR	3.7
1	A	388	GLY	3.7
1	A	272	GLY	3.6
1	A	421	GLY	3.5
1	A	487	LYS	3.5
1	A	259	ALA	3.0
1	A	442	PRO	2.9
1	A	460	THR	2.9
1	A	246	LYS	2.9
1	A	250	THR	2.8
1	A	390	CYS	2.7
1	A	422	PRO	2.7
1	A	389	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	441	PRO	2.6
1	A	448	PRO	2.6
1	A	445	ASN	2.6
1	A	298	MET	2.5
1	A	264	PHE	2.5
1	A	450	ARG	2.5
1	A	248	LYS	2.4
1	A	290	LEU	2.4
1	A	424	VAL	2.4
1	A	464	GLN	2.3
1	A	462	GLU	2.3
1	A	466	PRO	2.2
1	A	276	ALA	2.2
1	A	287	LYS	2.2
1	A	273	GLN	2.2
1	A	255	ILE	2.2
1	A	270	ALA	2.1
1	A	260	SER	2.1
1	A	427	TRP	2.1
1	A	323	MET	2.1
1	A	457	THR	2.1
1	A	262	THR	2.1
1	A	468	LYS	2.1
1	A	392	GLN	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($\text{\AA}^2$)	Q<0.9
2	CIT	A	602	13/13	0.66	0.19	76,88,123,132	0
3	SO4	A	603	5/5	0.72	0.11	99,111,117,117	5
2	CIT	A	601	13/13	0.89	0.13	60,93,129,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.