



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:21 AM UTC

PDB ID : 5R8W / pdb_00005r8w
Title : PanDDA analysis group deposition Form1 MAP kinase p38-alpha – Fragment K00283c in complex with MAP kinase p38-alpha
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Deposited on : 2020-03-04
Resolution : 1.50 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

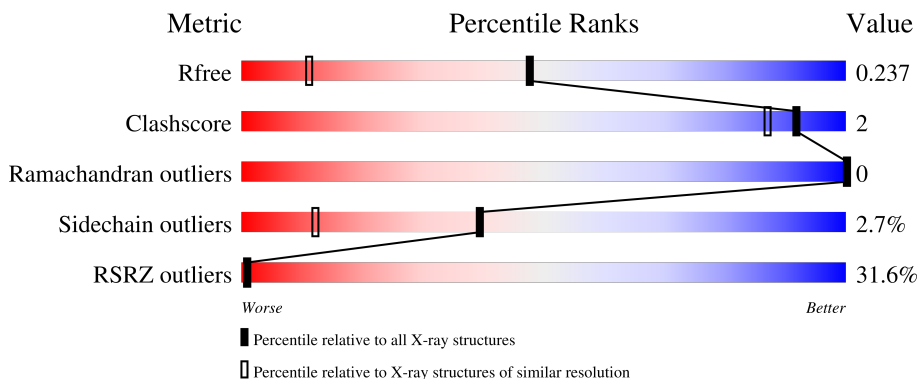
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	360	31% 88% 8% .

2 Entry composition [i](#)

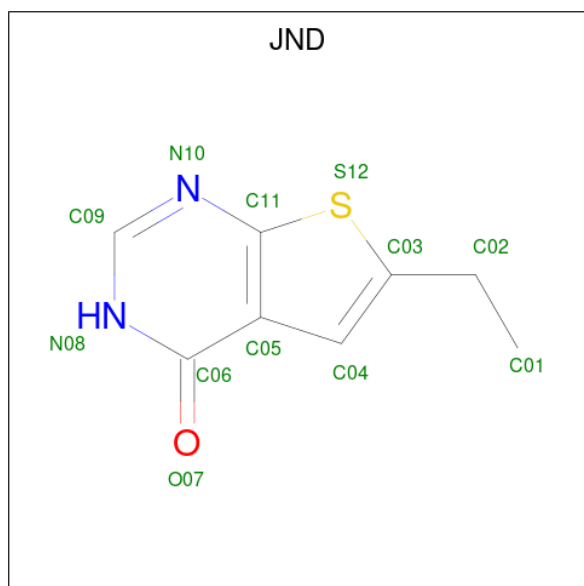
There are 7 unique types of molecules in this entry. The entry contains 3042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	3	0
			2773	1776	468	515	14			

- Molecule 2 is 6-ethylthieno[2,3-d]pyrimidin-4(3H)-one (CCD ID: JND) (formula: C₈H₈N₂OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	8	2	1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	Cl	0	0
			5	5		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

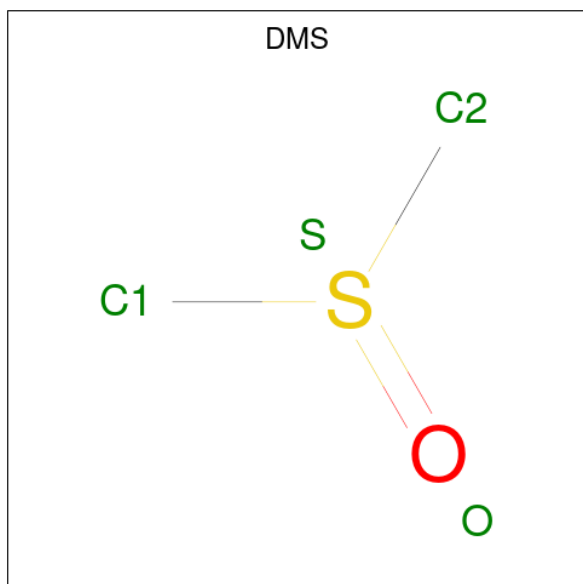
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

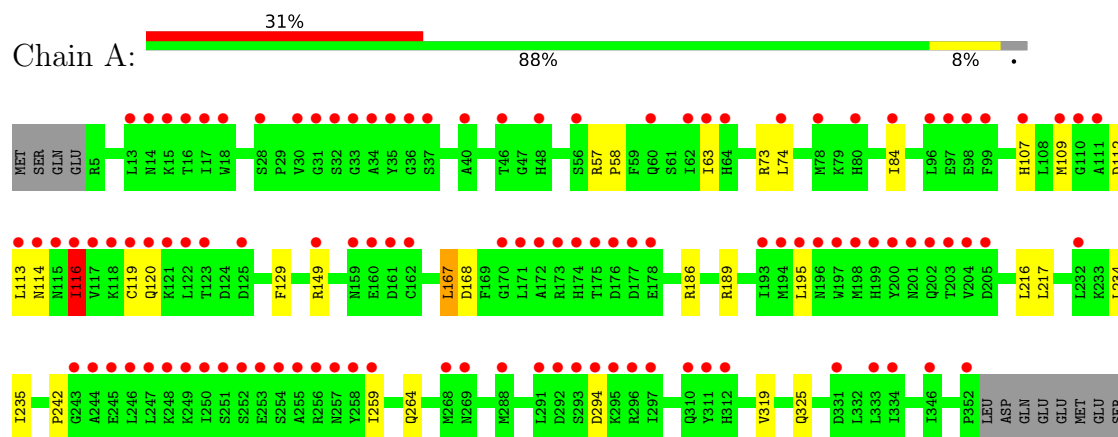
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	242	Total	O	0	0
			242	242		

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: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.78Å 86.10Å 127.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.36 – 1.50 71.36 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.36-1.50) 99.5 (71.36-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.185 , 0.201 0.237 , 0.237	Depositor DCC
R_{free} test set	4044 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	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	0.92	EDS
Total number of atoms	3042	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: DMS, MG, SO4, JND, CL

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	1.33	8/2839 (0.3%)	1.28	3/3863 (0.1%)

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	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	VAL	C-O	5.99	1.29	1.23
1	A	217	LEU	C-O	5.53	1.30	1.24
1	A	216	LEU	C-O	5.49	1.31	1.24
1	A	129	PHE	C-O	5.42	1.30	1.24
1	A	234	LEU	C-O	5.36	1.30	1.24
1	A	264	GLN	C-O	5.34	1.30	1.23
1	A	235	ILE	C-O	5.26	1.30	1.24
1	A	73	ARG	C-O	5.16	1.30	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ILE	CA-C-N	-5.57	111.94	121.97
1	A	116	ILE	C-N-CA	-5.57	111.94	121.97
1	A	325	GLN	CB-CA-C	-5.08	102.95	111.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ILE	Mainchain
1	A	186	ARG	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	2773	0	2694	9	0
2	A	12	0	0	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
6	A	4	0	6	0	0
7	A	242	0	0	2	0
All	All	3042	0	2700	9	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 (9) 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:84:ILE:HD13	1:A:109:MET:HE3	1.71	0.72
1:A:107:HIS:HD2	7:A:627:HOH:O	1.82	0.61
1:A:84:ILE:CD1	1:A:109:MET:HE3	2.36	0.55
1:A:294:ASP:OD1	7:A:501:HOH:O	2.18	0.54
1:A:149[A]:ARG:O	1:A:189:ARG:NH2	2.46	0.49
1:A:242:PRO:HG2	1:A:259:ILE:HG21	1.98	0.46
1:A:167:LEU:HD12	1:A:168:ASP:CG	2.42	0.45
1:A:112:ASP:OD1	1:A:114:ASN:HB2	2.18	0.43
1:A:57:ARG:N	1:A:58:PRO:CD	2.84	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	349/360 (97%)	336 (96%)	13 (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	294/319 (92%)	286 (97%)	8 (3%)	39	12

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

Mol	Chain	Res	Type
1	A	63	ILE
1	A	74	LEU
1	A	113	LEU
1	A	116	ILE
1	A	119	CYS
1	A	120	GLN
1	A	167	LEU
1	A	195	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	60	GLN
1	A	77	HIS
1	A	115	ASN
1	A	128	GLN
1	A	201	ASN
1	A	272	ASN
1	A	310	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	JND	A	401	-	13,13,13	1.08	0	15,18,18	2.27	3 (20%)
6	DMS	A	409	-	3,3,3	0.24	0	3,3,3	0.03	0
5	SO4	A	408	-	4,4,4	0.32	0	6,6,6	0.42	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	JND	A	401	-	-	0/2/2/2	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	401	JND	C05-C11-S12	6.22	114.80	111.17
2	A	401	JND	C09-N08-C06	-3.40	120.43	125.09
2	A	401	JND	C03-S12-C11	-3.23	89.65	91.35

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	348/360 (96%)	2.78	110 (31%) 1 1	3, 23, 45, 90	64 (18%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	THR	19.0
1	A	116	ILE	18.0
1	A	172	ALA	16.6
1	A	258	TYR	15.5
1	A	232	LEU	15.2
1	A	297	ILE	15.1
1	A	171	LEU	14.6
1	A	291	LEU	14.3
1	A	193	ILE	14.3
1	A	204	VAL	13.5
1	A	122	LEU	13.5
1	A	174	HIS	13.4
1	A	123	THR	12.4
1	A	149[A]	ARG	12.4
1	A	173	ARG	12.3
1	A	177	ASP	12.3
1	A	119	CYS	12.2
1	A	113	LEU	11.9
1	A	255	ALA	11.7
1	A	254	SER	11.7
1	A	120	GLN	11.6
1	A	247	LEU	11.5
1	A	195	LEU	11.2
1	A	115	ASN	11.1
1	A	244	ALA	11.0
1	A	294	ASP	10.7
1	A	250	ILE	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	197	TRP	10.5
1	A	293	SER	10.5
1	A	194	MET	10.2
1	A	246	LEU	10.2
1	A	176	ASP	10.2
1	A	257	ASN	10.1
1	A	205	ASP	10.1
1	A	203	THR	10.1
1	A	199	HIS	10.0
1	A	243	GLY	10.0
1	A	118	LYS	9.6
1	A	114	ASN	9.6
1	A	295	LYS	9.4
1	A	121	LYS	9.1
1	A	201	ASN	9.0
1	A	200	TYR	9.0
1	A	249	LYS	8.8
1	A	296	ARG	8.7
1	A	178	GLU	8.4
1	A	292	ASP	8.4
1	A	117	VAL	8.3
1	A	202	GLN	8.3
1	A	252	SER	8.2
1	A	288[A]	MET	8.0
1	A	253	GLU	8.0
1	A	248	LYS	7.9
1	A	256	ARG	7.9
1	A	312	HIS	7.7
1	A	198	MET	7.7
1	A	125[A]	ASP	7.7
1	A	196	ASN	7.6
1	A	31	GLY	7.4
1	A	80	HIS	7.2
1	A	245	GLU	6.8
1	A	268	MET	6.8
1	A	251	SER	6.5
1	A	33	GLY	6.5
1	A	78	MET	6.4
1	A	35	TYR	6.3
1	A	269	ASN	6.2
1	A	34	ALA	6.1
1	A	30	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	352	PRO	5.2
1	A	16	THR	5.0
1	A	13	LEU	4.9
1	A	32	SER	4.5
1	A	162	CYS	4.3
1	A	310	GLN	4.2
1	A	14	ASN	4.2
1	A	17	ILE	4.0
1	A	170	GLY	3.9
1	A	36	GLY	3.7
1	A	56	SER	3.6
1	A	331	ASP	3.6
1	A	346	ILE	3.6
1	A	63	ILE	3.5
1	A	109	MET	3.5
1	A	48	HIS	3.4
1	A	74	LEU	3.4
1	A	160	GLU	3.2
1	A	99	PHE	3.0
1	A	161	ASP	2.9
1	A	64	HIS	2.8
1	A	259	ILE	2.8
1	A	98	GLU	2.7
1	A	15	LYS	2.7
1	A	97	GLU	2.7
1	A	159	ASN	2.6
1	A	110	GLY	2.6
1	A	18	TRP	2.5
1	A	84	ILE	2.5
1	A	111	ALA	2.5
1	A	37	SER	2.4
1	A	333	LEU	2.3
1	A	62	ILE	2.3
1	A	334	ILE	2.3
1	A	60	GLN	2.3
1	A	107	HIS	2.3
1	A	96	LEU	2.3
1	A	40	ALA	2.2
1	A	311	TYR	2.0
1	A	46	THR	2.0
1	A	28	SER	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
6	DMS	A	409	4/4	0.71	0.37	83,84,95,97	0
2	JND	A	401	12/12	0.74	0.27	20,22,23,24	12
5	SO4	A	408	5/5	0.78	0.20	49,51,61,61	0
3	CL	A	404	1/1	0.94	0.16	48,48,48,48	0
3	CL	A	405	1/1	0.96	0.21	38,38,38,38	0
3	CL	A	402	1/1	0.97	0.37	42,42,42,42	0
3	CL	A	406	1/1	0.97	0.16	33,33,33,33	0
3	CL	A	403	1/1	0.98	0.10	36,36,36,36	0
4	MG	A	407	1/1	0.98	0.24	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.