



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:38 PM GMT

PDB ID : 3MVM
Title : P38 Alpha Map Kinase complexed with pyrrolotriazine inhibitor 7V
Authors : Sack, J.S.
Deposited on : 2010-05-04
Resolution : 2.00 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

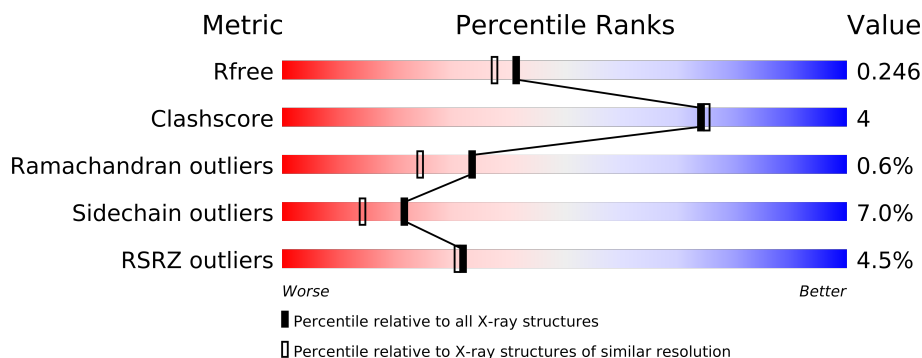
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	366	
1	B	366	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5829 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

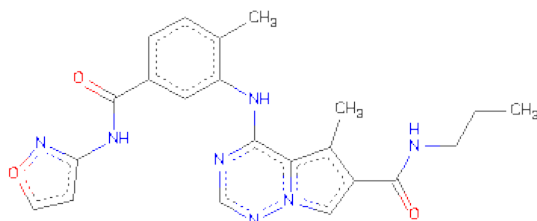
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2718	1743	467	496	12			
1	B	332	Total	C	N	O	S	0	0	0
			2697	1732	462	491	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q16539
A	-4	ALA	-	EXPRESSION TAG	UNP Q16539
A	-3	HIS	-	EXPRESSION TAG	UNP Q16539
A	-2	HIS	-	EXPRESSION TAG	UNP Q16539
A	-1	HIS	-	EXPRESSION TAG	UNP Q16539
A	0	HIS	-	EXPRESSION TAG	UNP Q16539
A	1	HIS	-	EXPRESSION TAG	UNP Q16539
B	-5	MET	-	EXPRESSION TAG	UNP Q16539
B	-4	ALA	-	EXPRESSION TAG	UNP Q16539
B	-3	HIS	-	EXPRESSION TAG	UNP Q16539
B	-2	HIS	-	EXPRESSION TAG	UNP Q16539
B	-1	HIS	-	EXPRESSION TAG	UNP Q16539
B	0	HIS	-	EXPRESSION TAG	UNP Q16539
B	1	HIS	-	EXPRESSION TAG	UNP Q16539

- Molecule 2 is 4-{[5-(ISOXAZOL-3-YLCARBAMOYL)-2-METHYLPHENYL]AMINO}-5-METHYL-N-PROPYLPYRROLO[2,1-F][1,2,4]TRIAZINE-6-CARBOXAMIDE (three-letter code: 39P) (formula: C₂₂H₂₃N₇O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 32	C 22	N 7	O 3	0	0
2	B	1	Total 32	C 22	N 7	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	162	Total O 162 162	0	0
3	B	188	Total O 188 188	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.31Å 71.34Å 72.53Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	24.48 – 2.00 24.48 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.48-2.00) 99.7 (24.48-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.99Å)	Xtriage
Refinement program	BUSTER 2.9.4	Depositor
R, R_{free}	0.197 , 0.238 0.201 , 0.246	Depositor DCC
R_{free} test set	2338 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
Estimated twinning fraction	0.002 for -h,l,k 0.017 for -h,-l,-k 0.032 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46361 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5829	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 39P

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	0.59	0/2780	0.74	2/3772 (0.1%)
1	B	0.60	0/2758	0.70	0/3741
All	All	0.60	0/5538	0.72	2/7513 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	THR	C-N-CA	5.62	135.75	121.70
1	A	104	LEU	CD1-CG-CD2	-5.04	95.39	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2718	0	2723	24	0
1	B	2697	0	2705	21	0
2	A	32	0	23	2	0
2	B	32	0	23	3	0
3	A	162	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	188	0	0	2	0
All	All	5829	0	5474	45	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:195:LEU:HD11	1:B:232:LEU:HD11	1.64	0.80
1:B:171:LEU:HD22	2:B:361:39P:H31	1.68	0.76
1:A:78:MET:HG3	1:A:140:TYR:HE2	1.54	0.73
1:A:238:LEU:HA	1:A:268:MET:HE2	1.75	0.68
1:B:27:LEU:HD23	1:B:41:ALA:HB2	1.77	0.66
1:A:109:MET:HG3	1:A:157:ALA:HB1	1.79	0.65
1:A:27:LEU:HD23	1:A:41:ALA:HB2	1.80	0.63
1:B:171:LEU:HD13	2:B:361:39P:H30	1.82	0.61
1:A:137:GLY:O	1:A:141:ILE:HG22	1.99	0.61
1:A:78:MET:HG3	1:A:140:TYR:CE2	2.36	0.60
1:A:138:LEU:HA	1:A:141:ILE:CG2	2.32	0.59
1:A:71:GLU:HB2	1:A:171:LEU:HD21	1.85	0.58
1:B:120:GLN:HG2	1:B:121:LYS:H	1.69	0.57
1:B:64:HIS:O	1:B:68:THR:HG23	2.05	0.57
1:A:174:HIS:CE1	1:A:193:ILE:HD13	2.40	0.56
1:A:23:ARG:O	1:A:44:THR:HB	2.06	0.55
1:B:23:ARG:O	1:B:44:THR:HB	2.07	0.54
1:A:197:TRP:HE1	1:A:259:ILE:HD11	1.74	0.53
1:A:238:LEU:HD12	1:A:268:MET:HE2	1.92	0.51
1:B:58:PRO:CB	1:B:68:THR:HG21	2.40	0.50
1:B:242:PRO:HB3	1:B:246:LEU:HD23	1.95	0.49
1:A:73:ARG:HE	1:A:77:HIS:CE1	2.32	0.48
1:A:117:VAL:HG21	1:A:216:LEU:CD2	2.44	0.48
1:B:62:ILE:HD12	1:B:334:ILE:HG13	1.96	0.47
1:A:109:MET:HG3	1:A:157:ALA:CB	2.42	0.47
1:B:242:PRO:HB2	1:B:247:LEU:HD13	1.96	0.47
1:A:185:THR:HB	1:A:186:ARG:H	1.44	0.45
1:B:108:LEU:HD23	1:B:108:LEU:C	2.36	0.45
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.99	0.45
1:A:173:ARG:O	1:A:175:THR:N	2.50	0.44
1:B:35:TYR:N	3:B:415:HOH:O	2.50	0.44
1:A:62:ILE:HD12	1:A:334:ILE:HG13	1.98	0.43
1:B:171:LEU:HD13	2:B:361:39P:C30	2.48	0.43
1:B:253:GLU:CD	1:B:256:ARG:HH22	2.21	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:LEU:HG	2:A:361:39P:C31	2.48	0.43
1:A:55:LEU:HD12	1:A:102:VAL:HG13	1.99	0.43
1:B:78:MET:CE	1:B:141:ILE:HA	2.49	0.43
1:A:235:ILE:HD11	3:A:448:HOH:O	2.19	0.42
1:B:55:LEU:HD12	1:B:102:VAL:HG13	2.03	0.41
1:B:35:TYR:HD1	3:B:397:HOH:O	2.02	0.41
1:A:71:GLU:HG3	2:A:361:39P:H31	2.02	0.41
1:B:192:GLU:HA	1:B:197:TRP:CD1	2.56	0.41
1:A:138:LEU:HA	1:A:141:ILE:HG22	2.02	0.40
1:B:186:ARG:HG3	1:B:194:MET:HE1	2.03	0.40
1:B:220:ARG:HB2	1:B:220:ARG:HE	1.71	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	329/366 (90%)	317 (96%)	8 (2%)	4 (1%)	19	9
1	B	326/366 (89%)	319 (98%)	7 (2%)	0	100	100
All	All	655/732 (90%)	636 (97%)	15 (2%)	4 (1%)	33	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ARG
1	A	118	LYS
1	A	263	THR
1	A	264	GLN

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	300/325 (92%)	277 (92%)	23 (8%)	18	11
1	B	297/325 (91%)	278 (94%)	19 (6%)	25	17
All	All	597/650 (92%)	555 (93%)	42 (7%)	21	14

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	44	THR
1	A	62	ILE
1	A	78	MET
1	A	108	LEU
1	A	141	ILE
1	A	151	LEU
1	A	162	CYS
1	A	173	ARG
1	A	185	THR
1	A	204	VAL
1	A	232	LEU
1	A	241	THR
1	A	247	LEU
1	A	251	SER
1	A	252	SER
1	A	262	LEU
1	A	275	ILE
1	A	285	LEU
1	A	291	LEU
1	A	293	SER
1	A	321	ASP
1	A	333	LEU
1	B	44	THR
1	B	62	ILE
1	B	79	LYS
1	B	108	LEU
1	B	113	LEU
1	B	119	CYS
1	B	145	ASP
1	B	151	LEU
1	B	197	TRP
1	B	199	HIS

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Mol	Chain	Res	Type
1	B	204	VAL
1	B	229	ILE
1	B	232	LEU
1	B	263	THR
1	B	269	ASN
1	B	275	ILE
1	B	285	LEU
1	B	293	SER
1	B	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	39P	A	361	-	35,35,35	1.97	8 (22%)	42,49,49	2.95	14 (33%)
2	39P	B	361	-	35,35,35	1.98	8 (22%)	42,49,49	2.97	16 (38%)

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	39P	A	361	-	-	0/18/20/20	0/2/4/4
2	39P	B	361	-	-	0/18/20/20	0/2/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	361	39P	N2-N1	6.75	1.45	1.36
2	A	361	39P	N2-N1	6.74	1.45	1.36
2	B	361	39P	C3-N4	3.64	1.41	1.33
2	A	361	39P	C3-N4	3.56	1.40	1.33
2	A	361	39P	C18-C19	3.45	1.46	1.40
2	B	361	39P	C18-C19	3.37	1.46	1.40
2	A	361	39P	C5-C6	3.22	1.51	1.44
2	B	361	39P	C6-N1	-3.21	1.36	1.40
2	A	361	39P	C6-N1	-3.21	1.36	1.40
2	B	361	39P	C5-C6	3.21	1.51	1.44
2	B	361	39P	C8-C7	2.90	1.46	1.41
2	A	361	39P	C8-C7	2.89	1.46	1.41
2	B	361	39P	C21-C22	2.50	1.43	1.39
2	A	361	39P	C21-C22	2.46	1.43	1.39
2	B	361	39P	C27-N26	-2.26	1.35	1.40
2	A	361	39P	C27-N26	-2.17	1.36	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	39P	C9-N1-N2	10.18	130.61	125.61
2	A	361	39P	C9-N1-N2	10.02	130.53	125.61
2	B	361	39P	C7-C6-N1	8.39	109.69	105.60
2	A	361	39P	C7-C6-N1	8.14	109.57	105.60
2	A	361	39P	C3-N4-C5	5.71	120.28	116.69
2	B	361	39P	C6-N1-N2	-5.62	120.44	126.95
2	A	361	39P	C6-N1-N2	-5.61	120.46	126.95
2	B	361	39P	C3-N4-C5	5.58	120.20	116.69
2	A	361	39P	N2-C3-N4	-4.82	119.24	127.85
2	B	361	39P	N2-C3-N4	-4.82	119.25	127.85
2	A	361	39P	C18-N17-C5	-3.73	118.91	128.79
2	B	361	39P	C18-N17-C5	-3.57	119.32	128.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	39P	C16-C7-C6	3.17	129.09	126.20
2	A	361	39P	C16-C7-C6	3.08	129.00	126.20
2	B	361	39P	C3-N2-N1	2.93	122.44	116.80
2	A	361	39P	C3-N2-N1	2.92	122.44	116.80
2	B	361	39P	O29-C30-C31	-2.86	109.29	111.53
2	B	361	39P	C9-C8-C7	2.83	106.70	103.90
2	A	361	39P	C9-C8-C7	2.81	106.67	103.90
2	A	361	39P	O29-C30-C31	-2.78	109.35	111.53
2	A	361	39P	C13-N12-C10	2.56	128.02	122.18
2	B	361	39P	C13-N12-C10	2.50	127.87	122.18
2	B	361	39P	C31-C27-N26	-2.48	124.97	129.76
2	A	361	39P	C31-C27-N26	-2.48	124.97	129.76
2	A	361	39P	O25-C24-C22	-2.40	116.80	121.01
2	A	361	39P	C23-C18-N17	-2.29	116.71	121.37
2	B	361	39P	O25-C24-C22	-2.28	117.00	121.01
2	B	361	39P	C23-C18-N17	-2.23	116.83	121.37
2	B	361	39P	C27-N26-C24	-2.06	122.71	128.16
2	B	361	39P	C8-C7-C6	-2.04	104.73	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	335/366 (91%)	0.34	19 (5%) 23 22	19, 34, 61, 72	0
1	B	332/366 (90%)	0.18	11 (3%) 44 44	15, 30, 55, 77	0
All	All	667/732 (91%)	0.26	30 (4%) 32 31	15, 32, 59, 77	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	TYR	7.4
1	B	199	HIS	5.9
1	B	14	ASN	3.6
1	A	97	GLU	3.6
1	A	226	THR	3.5
1	A	119	CYS	3.4
1	A	115	ASN	3.3
1	A	4	GLU	3.2
1	B	120	GLN	2.9
1	A	304	ALA	2.8
1	B	48	LEU	2.8
1	A	321	ASP	2.8
1	A	314	PRO	2.8
1	B	36	GLY	2.7
1	B	119	CYS	2.6
1	B	172	ALA	2.5
1	A	263	THR	2.5
1	A	131	ILE	2.4
1	A	322	PRO	2.4
1	A	110	GLY	2.3
1	A	14	ASN	2.3
1	A	77	HIS	2.3
1	A	134	ILE	2.2
1	A	198	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	352	PRO	2.1
1	B	16	THR	2.1
1	A	186	ARG	2.1
1	B	121	LYS	2.1
1	A	316	ASP	2.0
1	B	185	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	39P	A	361	32/32	0.13	-0.05	19,27,44,45	0
2	39P	B	361	32/32	0.13	-0.27	15,25,39,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.