



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2017 – 01:30 AM EDT

PDB ID : 2O8G  
Title : Rat pp1c gamma complexed with mouse inhibitor-2  
Authors : Hurley, T.D.  
Deposited on : unknown  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

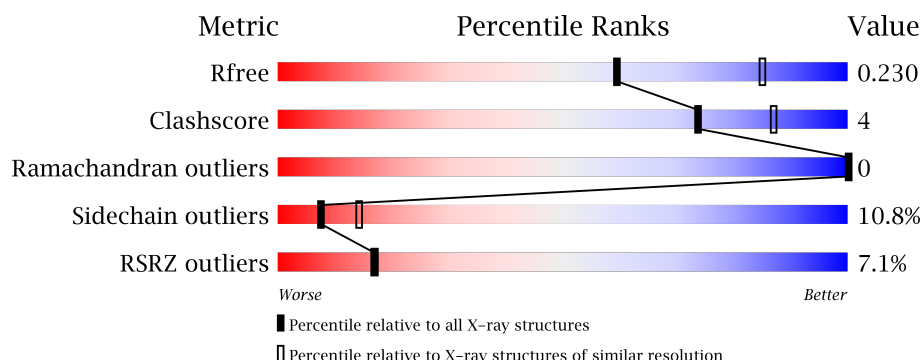
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	329	<div> <div>0.5%</div> <div>74%</div> <div>15%</div> <div>10%</div> </div>
1	B	329	<div> <div>0.5%</div> <div>74%</div> <div>15%</div> <div>10%</div> </div>
2	I	206	<div> <div>13%</div> <div>20%</div> <div>7%</div> <div>71%</div> </div>
2	J	206	<div> <div>9%</div> <div>17%</div> <div>10%</div> <div>72%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5987 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 phosphatase PP1-gamma catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2380	1527	399	436	18			
1	B	295	Total	C	N	O	S	0	0	0
			2380	1527	399	436	18			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	INITIATING METHIONINE	UNP P63088
A	-4	HIS	-	EXPRESSION TAG	UNP P63088
A	-3	HIS	-	EXPRESSION TAG	UNP P63088
A	-2	HIS	-	EXPRESSION TAG	UNP P63088
A	-1	HIS	-	EXPRESSION TAG	UNP P63088
A	0	HIS	-	EXPRESSION TAG	UNP P63088
A	1	HIS	-	EXPRESSION TAG	UNP P63088
B	-5	MET	-	INITIATING METHIONINE	UNP P63088
B	-4	HIS	-	EXPRESSION TAG	UNP P63088
B	-3	HIS	-	EXPRESSION TAG	UNP P63088
B	-2	HIS	-	EXPRESSION TAG	UNP P63088
B	-1	HIS	-	EXPRESSION TAG	UNP P63088
B	0	HIS	-	EXPRESSION TAG	UNP P63088
B	1	HIS	-	EXPRESSION TAG	UNP P63088

- Molecule 2 is a protein called Protein phosphatase inhibitor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	59	Total	C	N	O	S	0	0	0
			495	309	93	91	2			
2	J	58	Total	C	N	O	S	0	0	0
			487	305	92	88	2			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mn 1	0	0
3	A	1	Total 1	Mn 1	0	0

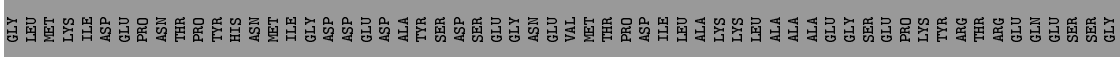
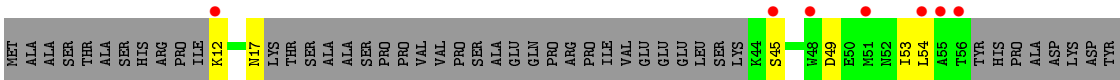
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total 111	O 111	0	0
4	I	18	Total 18	O 18	0	0
4	B	99	Total 99	O 99	0	0
4	J	15	Total 15	O 15	0	0



GLN  
HIS  
LYS  
SER  
GLN  
SER  
SER

• Molecule 2: Protein phosphatase inhibitor 2



GLN  
HIS  
LYS  
SER  
GLN  
SER  
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.27Å 103.23Å 149.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.50 48.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.80-2.50) 99.3 (48.81-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.235 0.190 , 0.230	Depositor DCC
$R_{free}$ test set	2622 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN

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	0.49	0/2434	0.77	7/3286 (0.2%)
1	B	0.47	0/2434	0.77	7/3286 (0.2%)
2	I	0.46	0/499	0.71	2/658 (0.3%)
2	J	0.48	0/491	0.69	1/647 (0.2%)
All	All	0.48	0/5858	0.76	17/7877 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ASP	CB-CG-OD2	7.49	125.04	118.30
1	A	92	ASP	CB-CG-OD2	7.12	124.71	118.30
1	B	286	ASP	CB-CG-OD2	6.95	124.56	118.30
1	B	92	ASP	CB-CG-OD2	6.64	124.28	118.30
2	J	168	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	208	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	138	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	166	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	240	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	253	ASP	CB-CG-OD2	5.46	123.22	118.30
2	I	169	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	138	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	240	ASP	CB-CG-OD2	5.37	123.13	118.30
2	I	165	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	166	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	208	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	277	ASP	CB-CG-OD2	5.07	122.86	118.30

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	2380	0	2351	16	0
1	B	2380	0	2351	20	0
2	I	495	0	507	2	0
2	J	487	0	503	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	111	0	0	4	0
4	B	99	0	0	4	0
4	I	18	0	0	2	0
4	J	15	0	0	2	0
All	All	5987	0	5712	43	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 4.

All (43) 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)
2:I:143:MET:HG2	4:I:222:HOH:O	2.00	0.61
2:J:132:PRO:HA	4:J:221:HOH:O	1.99	0.61
1:B:131:ASN:HB3	1:B:149:TRP:HE1	1.70	0.56
1:A:94:VAL:O	1:A:95:ASP:HB2	2.06	0.55
1:A:131:ASN:HB3	1:A:149:TRP:HE1	1.74	0.52
1:A:7:LEU:HD23	1:A:9:ILE:HD11	1.93	0.51
1:A:84:GLU:HB2	4:A:431:HOH:O	2.09	0.51
1:B:36:ARG:HG3	1:B:151:THR:HG21	1.93	0.51
1:B:198:GLN:HG2	4:B:357:HOH:O	2.12	0.49
1:B:94:VAL:O	1:B:95:ASP:HB2	2.13	0.49
1:B:96:ARG:HD3	4:B:359:HOH:O	2.13	0.47
1:B:257:PHE:CG	1:B:261:ARG:HG3	2.49	0.47
1:A:239:HIS:HD2	4:A:427:HOH:O	1.97	0.47
1:B:236:LEU:CD1	1:B:262:GLN:HB3	2.46	0.46
2:I:156:LYS:HE2	4:I:223:HOH:O	2.16	0.46
1:B:89:PHE:HB2	1:B:120:LEU:HD23	1.98	0.45
1:A:15:ARG:HH22	1:A:34:GLU:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HD11	1:A:89:PHE:CD2	2.51	0.45
1:B:239:HIS:HE1	4:B:336:HOH:O	2.00	0.45
1:B:218:GLU:HA	4:B:341:HOH:O	2.16	0.45
1:B:57:ALA:HB1	1:B:58:PRO:HA	1.99	0.45
2:J:167:HIS:CG	2:J:167:HIS:O	2.70	0.45
1:A:177:SER:HB2	1:A:203:ASP:HB2	1.99	0.44
2:J:17:ASN:HA	4:J:217:HOH:O	2.17	0.44
1:A:60:LYS:HZ3	1:A:284:SER:HG	1.65	0.44
1:A:290:MET:HE2	4:A:433:HOH:O	2.17	0.44
1:B:216:TRP:CZ3	1:B:227:PHE:HB3	2.52	0.44
1:B:70:TYR:CE2	1:B:74:ARG:HD2	2.53	0.43
1:A:57:ALA:HB1	1:A:58:PRO:HA	2.01	0.43
1:B:60:LYS:HZ2	1:B:294:GLN:HE22	1.66	0.42
1:B:60:LYS:NZ	1:B:294:GLN:HE22	2.17	0.42
1:A:23:LYS:HG3	4:A:429:HOH:O	2.19	0.42
1:B:266:LEU:HD21	1:B:283:MET:HB2	2.02	0.42
1:B:15:ARG:NH2	1:B:34:GLU:OE2	2.48	0.41
2:J:131:SER:HB3	2:J:134:GLU:HB2	2.01	0.41
1:A:255:TYR:HA	1:A:265:THR:O	2.21	0.41
1:A:113:LYS:HG2	1:A:114:TYR:CE1	2.56	0.41
1:B:15:ARG:HH22	1:B:34:GLU:CD	2.23	0.40
1:B:45:ILE:O	1:B:49:GLN:HG3	2.21	0.40
2:J:49:ASP:O	2:J:53:ILE:HG12	2.20	0.40
1:B:51:ILE:HD11	1:B:161:ILE:HD13	2.03	0.40
1:A:75:LEU:HD11	1:A:268:SER:HB3	2.03	0.40
1:A:6:LYS:HD2	1:A:6:LYS:HA	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	293/329 (89%)	279 (95%)	14 (5%)	0	100	100
1	B	293/329 (89%)	277 (94%)	16 (6%)	0	100	100
2	I	53/206 (26%)	53 (100%)	0	0	100	100
2	J	52/206 (25%)	51 (98%)	1 (2%)	0	100	100
All	All	691/1070 (65%)	660 (96%)	31 (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	261/291 (90%)	241 (92%)	20 (8%)	15	28
1	B	261/291 (90%)	244 (94%)	17 (6%)	20	37
2	I	54/181 (30%)	39 (72%)	15 (28%)	0	0
2	J	53/181 (29%)	37 (70%)	16 (30%)	0	0
All	All	629/944 (67%)	561 (89%)	68 (11%)	7	14

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	17	LEU
1	A	26	LYS
1	A	31	GLN
1	A	77	GLU
1	A	78	TYR
1	A	96	ARG
1	A	116	GLU
1	A	132	ARG
1	A	141	LYS
1	A	142	ARG
1	A	147	LYS
1	A	154	ASP

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Mol	Chain	Res	Type
1	A	161	ILE
1	A	198	GLN
1	A	211	LYS
1	A	246	ARG
1	A	260	LYS
1	A	284	SER
1	A	300	GLU
2	I	12	LYS
2	I	44	LYS
2	I	47	LYS
2	I	133	GLU
2	I	135	ARG
2	I	138	LYS
2	I	142	GLU
2	I	156	LYS
2	I	159	ARG
2	I	163	SER
2	I	164	LYS
2	I	165	ASP
2	I	166	LEU
2	I	167	HIS
2	I	168	ASP
1	B	6	LYS
1	B	14	GLN
1	B	23	LYS
1	B	26	LYS
1	B	77	GLU
1	B	78	TYR
1	B	96	ARG
1	B	116	GLU
1	B	142	ARG
1	B	161	ILE
1	B	211	LYS
1	B	218	GLU
1	B	246	ARG
1	B	261	ARG
1	B	284	SER
1	B	297	LYS
1	B	300	GLU
2	J	12	LYS
2	J	45	SER
2	J	54	LEU

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Mol	Chain	Res	Type
2	J	133	GLU
2	J	137	LYS
2	J	138	LYS
2	J	139	ARG
2	J	142	GLU
2	J	143	MET
2	J	144	LYS
2	J	153	LEU
2	J	156	LYS
2	J	164	LYS
2	J	165	ASP
2	J	167	HIS
2	J	168	ASP

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

Mol	Chain	Res	Type
1	A	27	ASN
1	A	239	HIS
1	A	294	GLN
2	I	140	GLN
1	B	99	GLN
1	B	181	GLN
1	B	239	HIS
1	B	294	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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	295/329 (89%)	-0.31	2 (0%) 87 88	31, 40, 59, 75	0
1	B	295/329 (89%)	-0.18	2 (0%) 87 88	32, 43, 63, 78	0
2	I	59/206 (28%)	2.08	27 (45%) 0 0	35, 69, 103, 103	0
2	J	58/206 (28%)	1.71	19 (32%) 0 0	34, 72, 100, 100	0
All	All	707/1070 (66%)	0.11	50 (7%) 17 17	31, 43, 90, 103	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	54	LEU	10.8
2	I	51	MET	8.2
2	I	56	THR	7.8
2	J	54	LEU	7.4
2	I	167	HIS	7.4
2	I	55	ALA	6.6
2	J	167	HIS	6.2
2	J	55	ALA	6.0
2	J	168	ASP	5.9
2	J	132	PRO	5.6
2	I	168	ASP	5.2
2	I	52	ASN	5.1
2	I	169	ASP	5.1
2	I	132	PRO	5.0
2	I	166	LEU	5.0
2	J	166	LEU	4.8
2	J	133	GLU	4.7
2	J	135	ARG	4.6
2	I	53	ILE	4.6
2	I	135	ARG	4.4
2	J	51	MET	4.3

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Mol	Chain	Res	Type	RSRZ
2	I	45	SER	4.2
1	A	300	GLU	4.2
2	J	134	GLU	4.1
2	J	56	THR	3.9
2	J	136	GLU	3.6
2	I	165	ASP	3.4
2	I	50	GLU	3.3
2	J	131	SER	3.2
2	J	12	LYS	3.2
2	I	49	ASP	3.0
2	I	134	GLU	3.0
2	I	48	TRP	3.0
1	B	300	GLU	3.0
2	I	47	LYS	2.8
2	I	46	GLN	2.7
2	J	164	LYS	2.6
2	J	139	ARG	2.4
2	I	12	LYS	2.4
2	I	164	LYS	2.4
2	J	130	LEU	2.4
2	I	133	GLU	2.4
1	A	23	LYS	2.2
2	I	136	GLU	2.2
2	J	45	SER	2.2
1	B	6	LYS	2.2
2	J	48	TRP	2.1
2	I	131	SER	2.1
2	I	44	LYS	2.1
2	I	130	LEU	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 [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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MN	B	324	1/1	1.00	0.05	-10.52	52,52,52,52	0
3	MN	A	324	1/1	0.99	0.04	-10.98	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.