



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:15 AM GMT

PDB ID : 2GCO
Title : Crystal structure of the human RhoC-GppNHp complex
Authors : Dias, S.M.G.; Cerione, R.A.
Deposited on : 2006-03-14
Resolution : 1.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

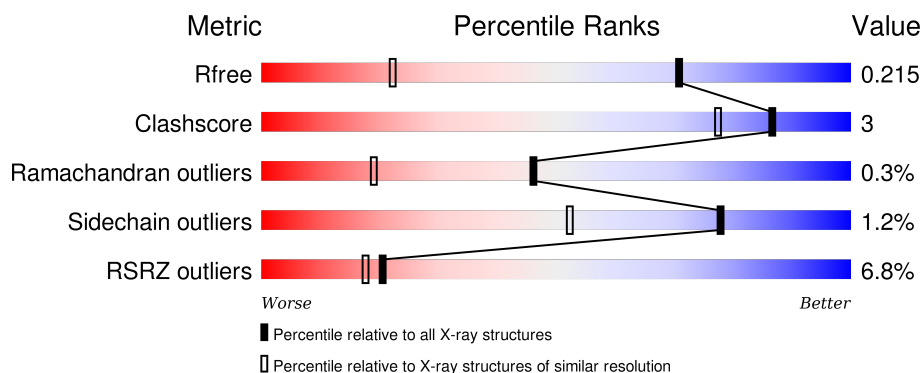
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	91344	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	201	 6% 88% 5% 6%
2	B	201	 6% 83% 8% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3573 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 Rho-related GTP-binding protein RhoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	7	0
			1528	966	264	289	9			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP P08134
A	-18	GLY	-	CLONING ARTIFACT	UNP P08134
A	-17	SER	-	CLONING ARTIFACT	UNP P08134
A	-16	SER	-	CLONING ARTIFACT	UNP P08134
A	-15	HIS	-	EXPRESSION TAG	UNP P08134
A	-14	HIS	-	EXPRESSION TAG	UNP P08134
A	-13	HIS	-	EXPRESSION TAG	UNP P08134
A	-12	HIS	-	EXPRESSION TAG	UNP P08134
A	-11	HIS	-	EXPRESSION TAG	UNP P08134
A	-10	HIS	-	EXPRESSION TAG	UNP P08134
A	-9	SER	-	CLONING ARTIFACT	UNP P08134
A	-8	SER	-	CLONING ARTIFACT	UNP P08134
A	-7	GLY	-	CLONING ARTIFACT	UNP P08134
A	-6	LEU	-	CLONING ARTIFACT	UNP P08134
A	-5	VAL	-	CLONING ARTIFACT	UNP P08134
A	-4	PRO	-	CLONING ARTIFACT	UNP P08134
A	-3	ARG	-	CLONING ARTIFACT	UNP P08134
A	-2	GLY	-	CLONING ARTIFACT	UNP P08134
A	-1	SER	-	CLONING ARTIFACT	UNP P08134
A	0	HIS	-	CLONING ARTIFACT	UNP P08134
A	107	CSX	CYS	MODIFIED RESIDUE	UNP P08134

- Molecule 2 is a protein called Rho-related GTP-binding protein RhoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	7	0
			1477	935	255	278	9			

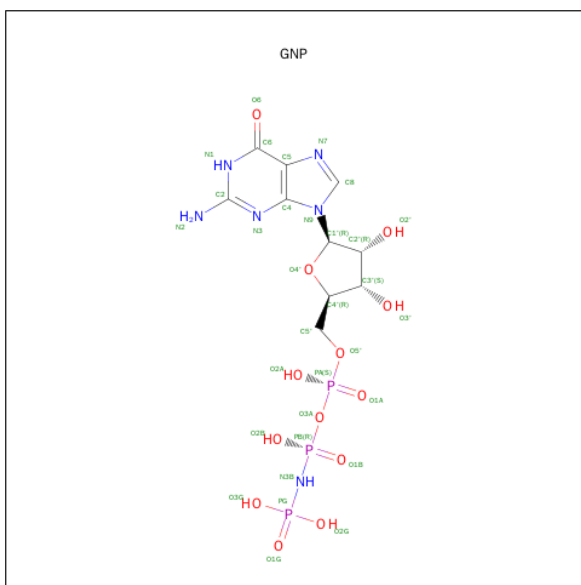
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	CLONING ARTIFACT	UNP P08134
B	-18	GLY	-	CLONING ARTIFACT	UNP P08134
B	-17	SER	-	CLONING ARTIFACT	UNP P08134
B	-16	SER	-	CLONING ARTIFACT	UNP P08134
B	-15	HIS	-	EXPRESSION TAG	UNP P08134
B	-14	HIS	-	EXPRESSION TAG	UNP P08134
B	-13	HIS	-	EXPRESSION TAG	UNP P08134
B	-12	HIS	-	EXPRESSION TAG	UNP P08134
B	-11	HIS	-	EXPRESSION TAG	UNP P08134
B	-10	HIS	-	EXPRESSION TAG	UNP P08134
B	-9	SER	-	CLONING ARTIFACT	UNP P08134
B	-8	SER	-	CLONING ARTIFACT	UNP P08134
B	-7	GLY	-	CLONING ARTIFACT	UNP P08134
B	-6	LEU	-	CLONING ARTIFACT	UNP P08134
B	-5	VAL	-	CLONING ARTIFACT	UNP P08134
B	-4	PRO	-	CLONING ARTIFACT	UNP P08134
B	-3	ARG	-	CLONING ARTIFACT	UNP P08134
B	-2	GLY	-	CLONING ARTIFACT	UNP P08134
B	-1	SER	-	CLONING ARTIFACT	UNP P08134
B	0	HIS	-	CLONING ARTIFACT	UNP P08134

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

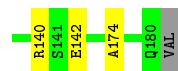


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	B	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	272	Total O 272 272	0	0
5	B	230	Total O 230 230	0	0

- Molecule 1: Rho-related GTP-binding protein RhoC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.09Å 75.64Å 82.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.40 8.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (8.00-1.40) 94.4 (8.00-1.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.219 0.194 , 0.215	Depositor DCC
R_{free} test set	3766 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 59.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 75014 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3573	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.49 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8494e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, GNP, CSX

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	0.41	0/1571	0.63	0/2120
2	B	0.43	0/1525	0.65	2/2057 (0.1%)
All	All	0.42	0/3096	0.64	2/4177 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	B	70	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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	1528	0	1537	7	0
2	B	1477	0	1497	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	13	0	0
4	B	32	0	13	0	0
5	A	272	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	230	0	0	1	0
All	All	3573	0	3060	16	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 3.

All (16) 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:33:VAL:HG23	1:A:34:TYR:H	1.45	0.80
1:A:37:THR:HG22	5:A:1077:HOH:O	1.95	0.67
2:B:80[A]:ILE:HD13	2:B:103:VAL:HG13	1.78	0.66
1:A:98:LYS:HE2	5:A:1117:HOH:O	2.02	0.58
2:B:80[A]:ILE:HD13	2:B:103:VAL:CG1	2.34	0.57
1:A:71:PRO:HA	1:A:74:TYR:CD2	2.45	0.51
1:A:33:VAL:HG23	1:A:34:TYR:N	2.22	0.50
2:B:80[A]:ILE:CD1	2:B:103:VAL:HG13	2.41	0.50
2:B:98:LYS:HE2	5:B:1109:HOH:O	2.12	0.49
1:A:124:ASP:N	5:A:1176:HOH:O	2.46	0.49
1:A:67:ASP:OD1	1:A:70[A]:ARG:NH2	2.30	0.48
2:B:71:PRO:HA	2:B:74:TYR:CD2	2.50	0.46
2:B:81:LEU:HD21	2:B:174:ALA:HB2	1.99	0.45
2:B:24:VAL:HG22	2:B:30:PHE:HA	2.00	0.44
2:B:140[A]:ARG:HD2	2:B:142:GLU:OE2	2.19	0.43
2:B:100:THR:O	2:B:104:LYS:HG2	2.20	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	190/201 (94%)	187 (98%)	2 (1%)	1 (0%)	34	10
2	B	183/201 (91%)	180 (98%)	3 (2%)	0	100	100
All	All	373/402 (93%)	367 (98%)	5 (1%)	1 (0%)	46	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	VAL

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	171/175 (98%)	169 (99%)	2 (1%)	78	52
2	B	168/176 (96%)	166 (99%)	2 (1%)	78	52
All	All	339/351 (97%)	335 (99%)	4 (1%)	78	52

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ASP
1	A	123	GLN
2	B	47	GLU
2	B	87	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
2	B	41	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSX	A	107	1	3,6,7	0.66	0	3,6,8	1.24	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
1	CSX	A	107	1	-	0/1/5/7	0/0/0/0

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.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
4	GNP	A	1001	3	28,34,34	1.90	7 (25%)	33,54,54	2.10	6 (18%)
4	GNP	B	1003	3	28,34,34	1.85	7 (25%)	33,54,54	1.99	6 (18%)

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
4	GNP	A	1001	3	-	0/12/38/38	0/3/3/3
4	GNP	B	1003	3	-	0/12/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	GNP	PB-O2B	-3.11	1.48	1.56
4	A	1001	GNP	PG-O2G	-2.87	1.48	1.56
4	A	1001	GNP	PB-O2B	-2.82	1.48	1.56
4	B	1003	GNP	PG-O2G	-2.33	1.50	1.56
4	A	1001	GNP	C8-N7	-2.32	1.30	1.34
4	B	1003	GNP	PB-O3A	-2.28	1.56	1.59
4	B	1003	GNP	C8-N7	-2.17	1.30	1.34
4	A	1001	GNP	PB-O3A	-2.00	1.56	1.59
4	A	1001	GNP	PB-O1B	2.53	1.49	1.46
4	B	1003	GNP	C6-N1	3.32	1.39	1.33
4	B	1003	GNP	PB-O1B	3.63	1.50	1.46
4	A	1001	GNP	C6-N1	3.91	1.40	1.33
4	B	1003	GNP	PG-O1G	6.04	1.53	1.46
4	A	1001	GNP	PG-O1G	6.56	1.53	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	GNP	C5-C6-N1	-8.15	112.44	123.59
4	B	1003	GNP	C5-C6-N1	-7.48	113.36	123.59
4	A	1001	GNP	O3G-PG-O1G	-3.48	104.24	113.49
4	B	1003	GNP	O3G-PG-O1G	-2.64	106.47	113.49
4	B	1003	GNP	O1G-PG-N3B	-2.38	108.25	111.90
4	A	1001	GNP	O1G-PG-N3B	-2.17	108.57	111.90
4	B	1003	GNP	O3G-PG-O2G	2.34	114.51	107.58
4	A	1001	GNP	O3G-PG-O2G	2.54	115.11	107.58
4	B	1003	GNP	O2B-PB-O1B	3.20	116.69	110.00
4	A	1001	GNP	O2B-PB-O1B	3.25	116.78	110.00
4	B	1003	GNP	C6-N1-C2	5.26	123.24	115.94
4	A	1001	GNP	C6-N1-C2	5.45	123.51	115.94

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	187/201 (93%)	0.10	12 (6%) 23 20	7, 11, 21, 30	20 (10%)
2	B	182/201 (90%)	0.12	13 (7%) 19 16	8, 12, 24, 28	13 (7%)
All	All	369/402 (91%)	0.11	25 (6%) 20 18	7, 11, 23, 30	33 (8%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	VAL	7.9
2	B	35	VAL	5.9
2	B	37	THR	5.5
1	A	2	ALA	4.8
1	A	34	TYR	4.5
2	B	28	ASP	4.5
1	A	-12	HIS	4.1
2	B	40	GLU	4.0
2	B	31	PRO	3.8
1	A	66	TYR	3.6
2	B	-4	PRO	3.5
1	A	68	ARG	3.2
1	A	-4	PRO	3.2
2	B	66	TYR	3.1
1	A	3	ALA	2.9
1	A	32	GLU	2.9
1	A	-7	GLY	2.9
2	B	42	TYR	2.6
2	B	41	ASN	2.5
1	A	65	ASP	2.3
2	B	30	PHE	2.3
2	B	39	PHE	2.3
1	A	123	GLN	2.2
2	B	38	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	68	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CSX	A	107	7/8	0.96	0.08	-	10,11,15,21	0

6.3 Carbohydrates [i](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	GNP	A	1001	32/32	0.97	0.08	0.45	9,11,16,16	0
4	GNP	B	1003	32/32	0.98	0.08	-0.24	10,12,15,17	0
3	MG	B	1004	1/1	0.99	0.06	-0.65	11,11,11,11	0
3	MG	A	1002	1/1	1.00	0.03	-2.41	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.