



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID : 1Z2C
Title : Crystal structure of mDIA1 GBD-FH3 in complex with RhoC-GMPPNP
Authors : Rose, R.; Weyand, M.; Lammers, M.; Ishizaki, T.; Ahmadian, M.R.; Wittinghofer, A.
Deposited on : 2005-03-08
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

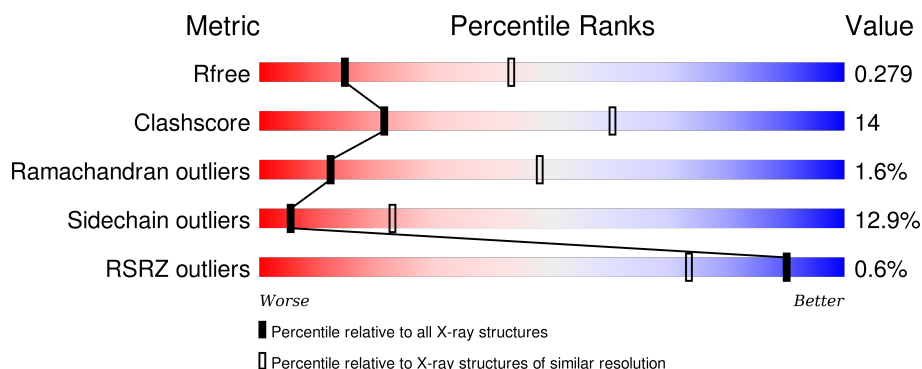
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



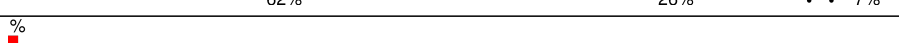

The reported resolution of this entry is 3.00 Å.

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	193	 61% 25% 6% • 7%
1	C	193	 62% 26% • • 7%
2	B	383	 60% 27% • 10%
2	D	383	 53% 28% 6% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8399 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	179	Total	C	N	O	S	0	0	0
			1419	894	242	273	10			
1	C	179	Total	C	N	O	S	0	0	0
			1416	892	242	273	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASN	PHE	ENGINEERED	UNP P08134
C	25	ASN	PHE	ENGINEERED	UNP P08134

- Molecule 2 is a protein called Diaphanous protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2788	1756	477	531	24			
2	D	335	Total	C	N	O	S	0	0	0
			2709	1712	461	512	24			

- 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		
3	C	1	Total	Mg	0	0
			1	1		

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

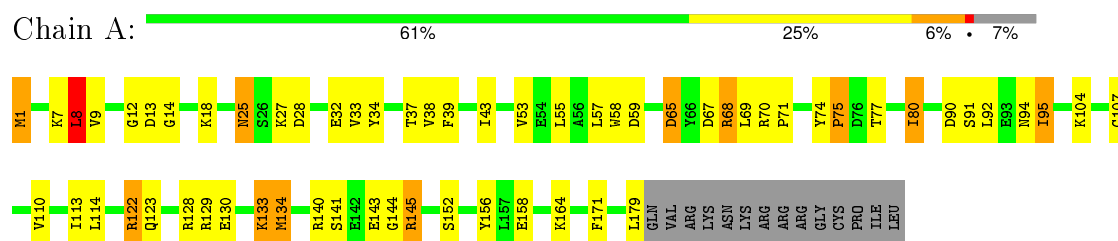


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	C	1	Total 32	C 10	N 6	O 13	P 3	0	0

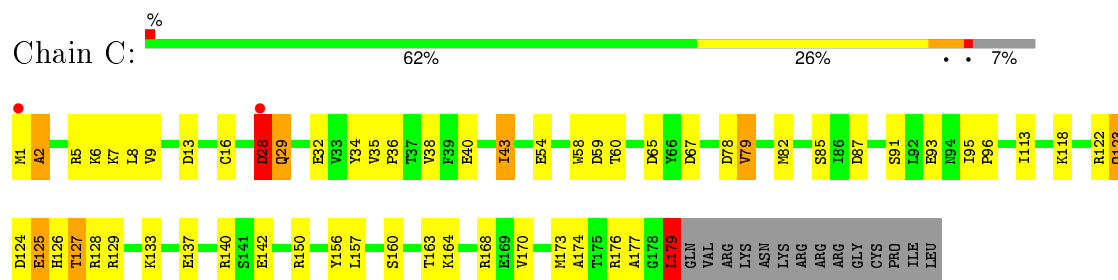
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

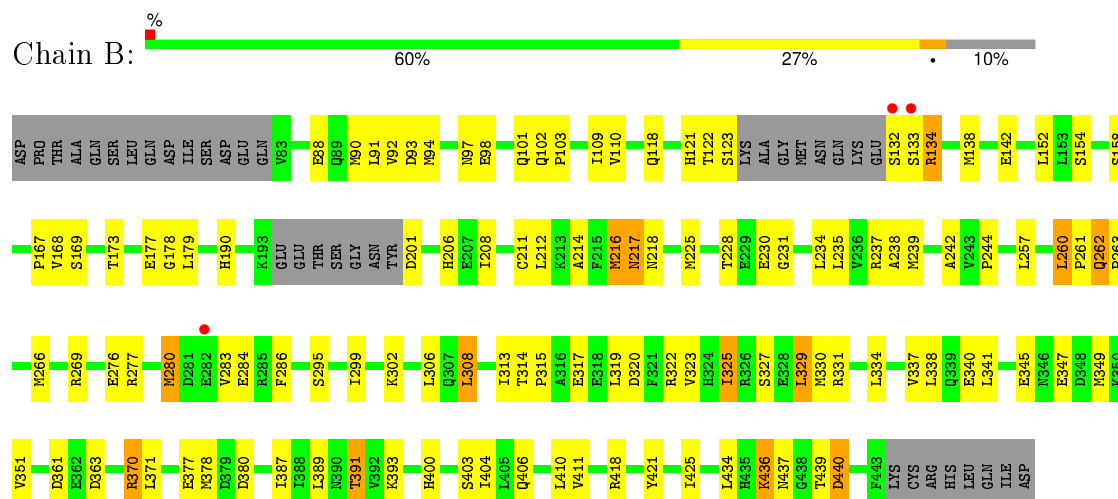
• Molecule 1: Rho-related GTP-binding protein RhoC



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



• Molecule 2: Diaphanous protein homolog 1



• Molecule 2: Diaphanous protein homolog 1

Chain D: 53% 28% 6% 13%

Q431 I432	K436	ASN GLY THR ASP	PRO ASP PHE LYS CYS ARG HIS LEU GLN ILE ASP	K223	T314 P315 A316	L319	R322 V323 H324	E328	R331	L332	G333	V337	E340	L341	R342	E343 I344 E345	N346 E347	C354	E358	D363	K368	L371	R375	K386 A397	E398 P399	L402	L405 Q406	L410 V411	R412 N413	P418 P419	L424 I425	E426	
				ARG SER A136	Y139 I140	R144	R148	L153 S154	L159 R160	N165	V168	Q172 T173	L179	L182 L183	L186 K187 R188 L189	H190 D191 E192	LYS GLY GLU THR	SER SER GLY ASN	V200 D201 S202	R203	I208 I209	R210 C211	L212 K213	M216 N217 N218	I222								
ASP	PRO	THR	ALA	GLN	SER	LEU	GLN	ASP	ASP	ILE	SER	ASP	GLU	GLN	V83 L84 V85 L86	F87 E88 Q89	M90 L91 V92	D93 M94 N95	E98	E99 K100	Q101 Q102 P103 L104	R105 E106 K107 D108	I109 V110	I111 K112 R113	E114	S117	T122	S123	LYS	ALA GLY MET	ASN GLN	LYS GLU SER	SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	148.64Å 85.35Å 123.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 100.0 (19.80-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.285 0.209 , 0.279	Depositor DCC
R_{free} test set	1605 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31996 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8399	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GNP, MG

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	0.71	0/1445	0.85	5/1953 (0.3%)
1	C	0.62	0/1442	0.74	1/1950 (0.1%)
2	B	0.78	3/2825 (0.1%)	0.83	1/3801 (0.0%)
2	D	0.87	3/2745 (0.1%)	0.86	3/3694 (0.1%)
All	All	0.77	6/8457 (0.1%)	0.83	10/11398 (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
2	B	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	107	LYS	CD-CE	20.83	2.03	1.51
2	D	107	LYS	CE-NZ	14.29	1.84	1.49
2	B	347	GLU	CG-CD	8.44	1.64	1.51
2	B	347	GLU	CB-CG	7.38	1.66	1.52
2	B	98	GLU	CG-CD	6.84	1.62	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	107	LYS	CD-CE-NZ	-11.82	84.51	111.70
2	D	107	LYS	CG-CD-CE	-7.66	88.91	111.90
1	A	68	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	B	329	LEU	CA-CB-CG	6.17	129.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	179	LEU	CA-CB-CG	5.86	128.79	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	216	MET	Peptide

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	1419	0	1415	36	0
1	C	1416	0	1409	51	0
2	B	2788	0	2811	71	0
2	D	2709	0	2739	84	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	32	0	13	2	0
4	C	32	0	13	2	0
All	All	8399	0	8400	238	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 14.

The worst 5 of 238 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:D:107:LYS:CE	2:D:107:LYS:NZ	1.84	1.38
2:D:107:LYS:CE	2:D:107:LYS:CD	2.03	1.35
2:B:262:GLN:HG3	2:B:263:PRO:HD3	1.20	1.12
2:D:91:LEU:HD22	2:D:101:GLN:HG3	1.41	1.02
1:C:140:ARG:HB2	1:C:140:ARG:NH1	1.81	0.96

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	177/193 (92%)	156 (88%)	18 (10%)	3 (2%)	11	46
1	C	177/193 (92%)	160 (90%)	14 (8%)	3 (2%)	11	46
2	B	340/383 (89%)	307 (90%)	28 (8%)	5 (2%)	13	50
2	D	329/383 (86%)	292 (89%)	32 (10%)	5 (2%)	13	50
All	All	1023/1152 (89%)	915 (89%)	92 (9%)	16 (2%)	12	48

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
2	B	122	THR
2	B	217	ASN
1	C	28	ASP
2	D	190	HIS

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	157/170 (92%)	135 (86%)	22 (14%)	4	19
1	C	156/170 (92%)	139 (89%)	17 (11%)	8	30
2	B	316/350 (90%)	280 (89%)	36 (11%)	7	28
2	D	306/350 (87%)	260 (85%)	46 (15%)	3	17
All	All	935/1040 (90%)	814 (87%)	121 (13%)	5	23

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	411	VAL
1	C	125	GLU
2	D	402	LEU
2	B	436	LYS
1	C	32	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	324	HIS
2	B	406	GLN
2	D	335	HIS
2	B	287	GLN
2	D	324	HIS

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 5 ligands modelled in this entry, 3 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	195	3	28,34,34	1.72	5 (17%)	33,54,54	2.50	9 (27%)
4	GNP	C	195	3	28,34,34	1.70	5 (17%)	33,54,54	2.61	11 (33%)

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	195	3	-	0/12/38/38	0/3/3/3
4	GNP	C	195	3	-	0/12/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	195	GNP	PB-O3A	-4.09	1.54	1.59
4	A	195	GNP	PB-O3A	-3.39	1.54	1.59
4	A	195	GNP	PB-O2B	-2.99	1.48	1.56
4	C	195	GNP	PB-O2B	-2.70	1.49	1.56
4	C	195	GNP	C8-N7	-2.16	1.30	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	195	GNP	C5-C6-N1	-8.80	111.56	123.59
4	C	195	GNP	C5-C6-N1	-8.52	111.93	123.59
4	A	195	GNP	O3G-PG-O1G	-4.46	101.65	113.49
4	C	195	GNP	C2'-C1'-N9	-4.17	107.92	114.29
4	C	195	GNP	O1B-PB-N3B	-3.62	106.34	111.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	195	GNP	2	0
4	C	195	GNP	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	179/193 (92%)	-0.48	0 100 100	28, 52, 93, 108	0
1	C	179/193 (92%)	-0.43	2 (1%) 82 58	35, 56, 100, 119	0
2	B	346/383 (90%)	-0.55	3 (0%) 85 64	26, 44, 76, 101	0
2	D	335/383 (87%)	-0.57	1 (0%) 94 84	21, 49, 78, 95	0
All	All	1039/1152 (90%)	-0.52	6 (0%) 90 73	21, 48, 85, 119	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	SER	2.8
2	B	282	GLU	2.6
1	C	28	ASP	2.3
2	B	133	SER	2.3
2	D	200	TYR	2.1

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 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(\AA^2)	Q<0.9
3	MG	A	194	1/1	0.95	0.18	0.75	31,31,31,31	0
3	MG	C	194	1/1	0.97	0.20	0.09	56,56,56,56	0
4	GNP	C	195	32/32	0.97	0.13	-0.68	49,57,61,61	0
4	GNP	A	195	32/32	0.96	0.13	-0.82	42,54,56,57	0
3	MG	B	5	1/1	0.94	0.44	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.