



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2017 – 05:52 PM EDT

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 : unknown
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 : 1.7.2 (RC1), CSD as538be (2017)
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

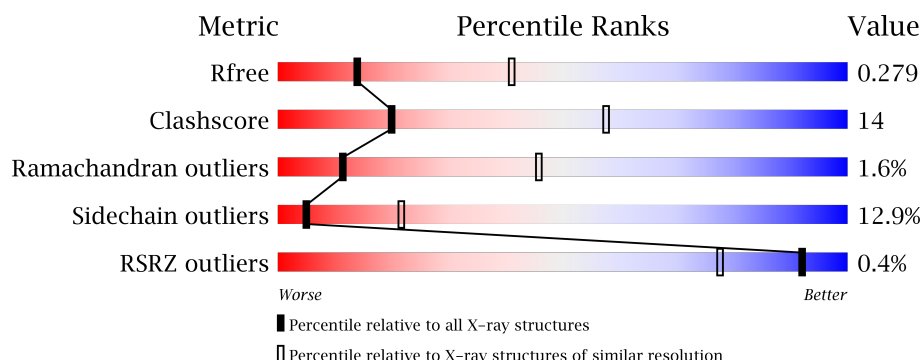
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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	
1	C	193	
2	B	383	
2	D	383	

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

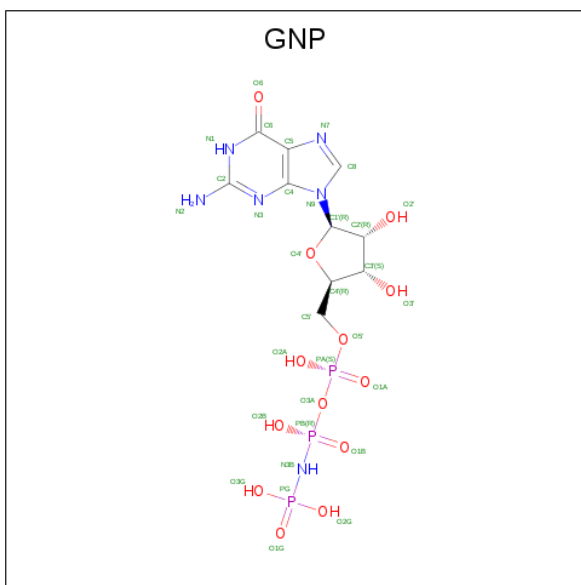
- Molecule 2 is a protein called Diaphanous protein homolog 1.

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).

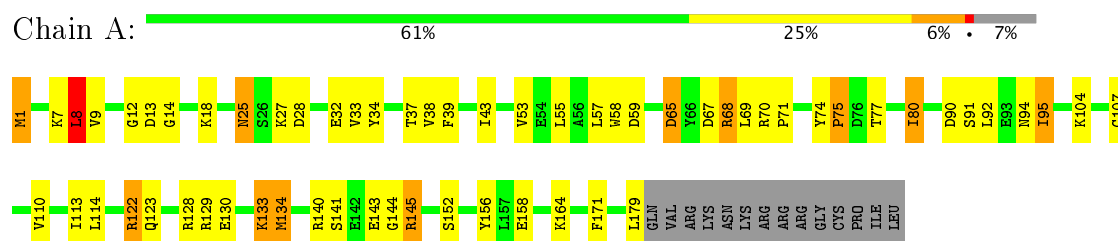


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	C	1	Total 32	C 10	N 6	O 13	P 3	0	0

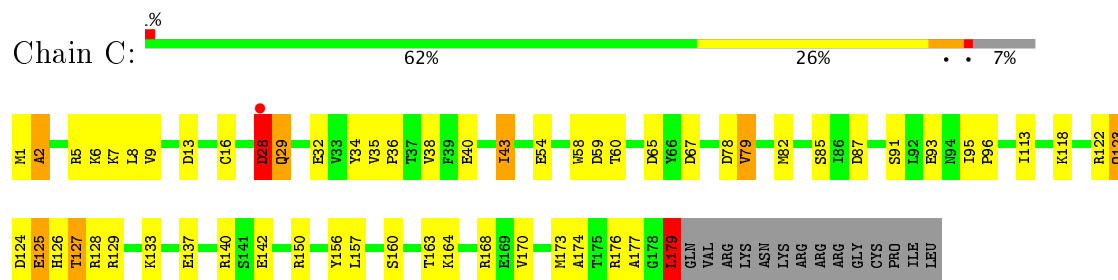
3 Residue-property plots

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

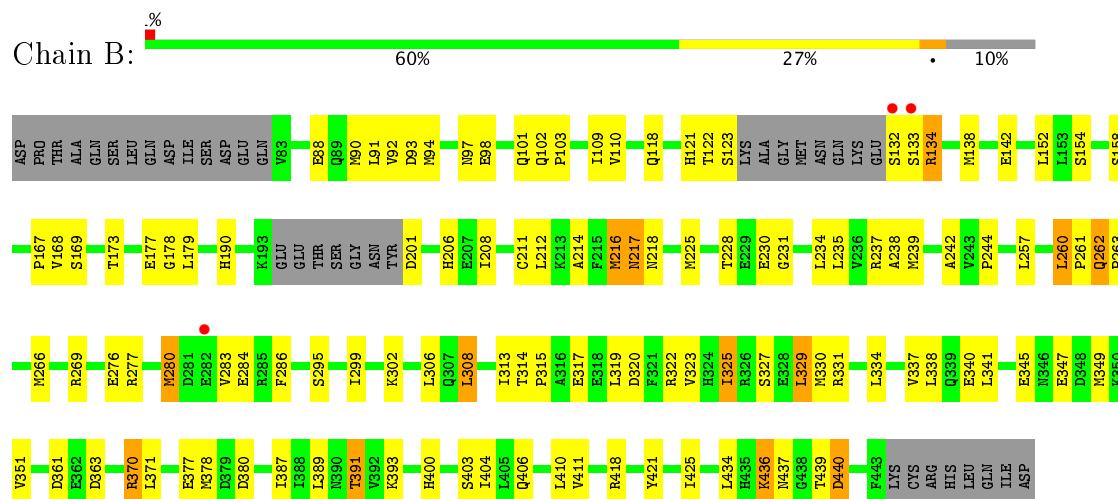
- Molecule 1: Rho-related GTP-binding protein RhoC



- 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%

ASP	PRQ	THR	ALA	GLN	SER	LEU	GLN	ASP	ASP	ASP	GLU	GLN	V83	L84	V85	L86	F87	E88	Q89	N90	L91	V92	D93	M94	N95	E98	E99	K100	Q101	Q102	P103	L104	R105	E106	K107	D108	V109	I110	I111	K112	R113	E114	S117	T122	S123	L125	ALA	GLY	MET	ASN	GLN	L125	GLU	SER
ARG	SER	A136	E227	Y139	I140	R144	R148	R237	L153	S154	L159	R160	N165	V168	Q172	T173	L179	L182	L183	L186	K187	R188	L189	H190	D191	E192	LVS	GLU	GLU	THR	SER	GLY	ASN	V200	D201	S202	R203	I208	I209	R210	C211	L212	R213	K216	R217	R218	I222							
K223	L226	E227	T228	E229	E230	G231	V236	R237	A238	M239	M247	I248	D249	A251	K252	L253	L254	S255	C258	I259	P261	Q262	P263	E264	D265	E268	R269	E272	A273	M274	R277	D281	E282	V283	E284	R285	L289	L290	L293	K294	L301	L308	A311											
T314	F315	A316	L319	R322	V323	H324	E328	R331	L332	G333	V337	E340	L341	R342	E343	I344	E345	R346	E347	C354	E358	D363	K368	L371	R375	K396	A397	E398	P399	L402	L405	Q406	I410	V411	R412	N413	R418	P419	L424	I425	E426													
Q431	I432	K436	ASN	GLY	THR	ASP	PRO	ASP	PHE	LYS	CYS	ARG	HIS	LEU	GLN	ILE	ASP																																					

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
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	0.93	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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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:NH1	1:C:140:ARG:HB2	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	44
1	C	177/193 (92%)	160 (90%)	14 (8%)	3 (2%)	11	44
2	B	340/383 (89%)	307 (90%)	28 (8%)	5 (2%)	12	48
2	D	329/383 (86%)	292 (89%)	32 (10%)	5 (2%)	12	48
All	All	1023/1152 (89%)	915 (89%)	92 (9%)	16 (2%)	11	46

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	18
1	C	156/170 (92%)	139 (89%)	17 (11%)	7	29
2	B	316/350 (90%)	280 (89%)	36 (11%)	7	27
2	D	306/350 (87%)	260 (85%)	46 (15%)	3	16
All	All	935/1040 (90%)	814 (87%)	121 (13%)	5	22

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	27,34,34	2.48	7 (25%)	26,54,54	1.75	4 (15%)
4	GNP	C	195	3	27,34,34	2.63	8 (29%)	26,54,54	1.97	8 (30%)

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	-	0/16/38/38	0/3/3/3
4	GNP	C	195	3	-	0/16/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	195	GNP	C4-N9	-7.33	1.38	1.47
4	C	195	GNP	C5-C6	-6.70	1.40	1.53
4	A	195	GNP	C4-N9	-6.48	1.39	1.47
4	A	195	GNP	C5-C6	-5.76	1.42	1.53
4	C	195	GNP	PB-O3A	-4.15	1.54	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	195	GNP	O3G-PG-O1G	-4.63	101.65	113.41
4	C	195	GNP	O3G-PG-O1G	-3.74	103.89	113.41
4	C	195	GNP	O1B-PB-N3B	-3.64	106.34	111.79
4	C	195	GNP	C2'-C1'-N9	-2.09	107.92	113.34
4	C	195	GNP	O3A-PB-N3B	2.15	112.56	106.59

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%)	-0.49	0 100 100	28, 52, 93, 108	0
1	C	179/193 (92%)	-0.45	1 (0%) 89 71	35, 56, 100, 119	0
2	B	346/383 (90%)	-0.56	3 (0%) 84 61	26, 44, 76, 101	0
2	D	335/383 (87%)	-0.58	0 100 100	21, 49, 78, 95	0
All	All	1039/1152 (90%)	-0.53	4 (0%) 92 77	21, 48, 85, 119	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	SER	2.7
2	B	282	GLU	2.6
1	C	28	ASP	2.2
2	B	133	SER	2.2

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.