W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 14, 2014 – 11:43 PM EDT

PDB ID	:	4PMW
Title	:	Structure of mouse Dis3L2 in complex with oligoU RNA substrate
Authors	:	Faehnle, C.R.; Walleshauser, J.; Joshua-Tor, L.
Deposited on	:	2014-05-22
Resolution	:	2.95 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.95 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	Percentile Ranks	Value
Rfree		0.251
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		0.5%
RSRZ outliers		4.7%
RNA backbone		0.37

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
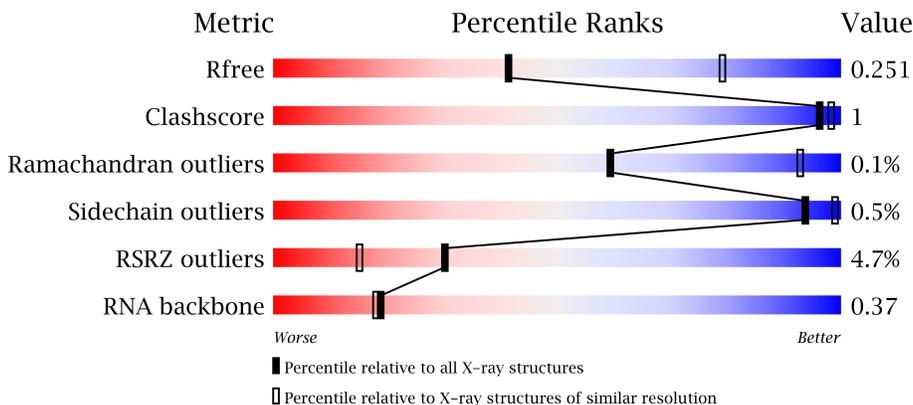
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)
RNA backbone	1838	1019 (3.46-2.46)

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	770	
1	B	770	
2	C	14	
2	D	14	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22942 atoms, of which 11358 are hydrogens 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 DIS3-like exonuclease 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	691	Total 11046	C 3518	H 5538	N 937	O 1022	S 31	0	0	0
1	B	691	Total 11046	C 3518	H 5538	N 937	O 1022	S 31	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP Q8CI75
A	?	-	HIS	deletion	UNP Q8CI75
A	?	-	PRO	deletion	UNP Q8CI75
A	?	-	LEU	deletion	UNP Q8CI75
A	?	-	GLN	deletion	UNP Q8CI75
A	?	-	GLN	deletion	UNP Q8CI75
A	?	-	SER	deletion	UNP Q8CI75
A	?	-	ARG	deletion	UNP Q8CI75
A	?	-	LYS	deletion	UNP Q8CI75
A	?	-	GLY	deletion	UNP Q8CI75
A	?	-	TRP	deletion	UNP Q8CI75
A	?	-	SER	deletion	UNP Q8CI75
A	?	-	GLY	deletion	UNP Q8CI75
A	?	-	PRO	deletion	UNP Q8CI75
A	?	-	ASP	deletion	UNP Q8CI75
A	?	-	VAL	deletion	UNP Q8CI75
A	?	-	ILE	deletion	UNP Q8CI75
A	?	-	ILE	deletion	UNP Q8CI75
A	?	-	GLU	deletion	UNP Q8CI75
A	?	-	ALA	deletion	UNP Q8CI75
A	?	-	GLN	deletion	UNP Q8CI75
A	?	-	PHE	deletion	UNP Q8CI75
A	?	-	SER	deletion	UNP Q8CI75
A	?	-	THR	deletion	UNP Q8CI75
A	?	-	PRO	deletion	UNP Q8CI75

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q8CI75
A	?	-	ARG	deletion	UNP Q8CI75
A	?	-	GLY	deletion	UNP Q8CI75
A	?	-	LYS	deletion	UNP Q8CI75
A	?	-	GLU	deletion	UNP Q8CI75
A	?	-	ASP	deletion	UNP Q8CI75
A	?	-	SER	deletion	UNP Q8CI75
A	?	-	SER	deletion	UNP Q8CI75
A	?	-	THR	deletion	UNP Q8CI75
A	?	-	PRO	deletion	UNP Q8CI75
A	?	-	VAL	deletion	UNP Q8CI75
A	?	-	MET	deletion	UNP Q8CI75
A	?	-	LYS	deletion	UNP Q8CI75
A	?	-	ASP	deletion	UNP Q8CI75
A	?	-	GLU	deletion	UNP Q8CI75
A	?	-	ASN	deletion	UNP Q8CI75
A	?	-	THR	deletion	UNP Q8CI75
A	?	-	PRO	deletion	UNP Q8CI75
A	?	-	ILE	deletion	UNP Q8CI75
A	?	-	PRO	deletion	UNP Q8CI75
A	?	-	GLN	deletion	UNP Q8CI75
A	?	-	ASP	deletion	UNP Q8CI75
A	?	-	THR	deletion	UNP Q8CI75
A	?	-	ARG	deletion	UNP Q8CI75
A	?	-	GLY	deletion	UNP Q8CI75
A	389	ASN	ASP	engineered mutation	UNP Q8CI75
B	?	-	HIS	deletion	UNP Q8CI75
B	?	-	HIS	deletion	UNP Q8CI75
B	?	-	PRO	deletion	UNP Q8CI75
B	?	-	LEU	deletion	UNP Q8CI75
B	?	-	GLN	deletion	UNP Q8CI75
B	?	-	GLN	deletion	UNP Q8CI75
B	?	-	SER	deletion	UNP Q8CI75
B	?	-	ARG	deletion	UNP Q8CI75
B	?	-	LYS	deletion	UNP Q8CI75
B	?	-	GLY	deletion	UNP Q8CI75
B	?	-	TRP	deletion	UNP Q8CI75
B	?	-	SER	deletion	UNP Q8CI75
B	?	-	GLY	deletion	UNP Q8CI75
B	?	-	PRO	deletion	UNP Q8CI75
B	?	-	ASP	deletion	UNP Q8CI75
B	?	-	VAL	deletion	UNP Q8CI75

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ILE	deletion	UNP Q8CI75
B	?	-	ILE	deletion	UNP Q8CI75
B	?	-	GLU	deletion	UNP Q8CI75
B	?	-	ALA	deletion	UNP Q8CI75
B	?	-	GLN	deletion	UNP Q8CI75
B	?	-	PHE	deletion	UNP Q8CI75
B	?	-	SER	deletion	UNP Q8CI75
B	?	-	THR	deletion	UNP Q8CI75
B	?	-	PRO	deletion	UNP Q8CI75
B	?	-	ASP	deletion	UNP Q8CI75
B	?	-	ARG	deletion	UNP Q8CI75
B	?	-	GLY	deletion	UNP Q8CI75
B	?	-	LYS	deletion	UNP Q8CI75
B	?	-	GLU	deletion	UNP Q8CI75
B	?	-	ASP	deletion	UNP Q8CI75
B	?	-	SER	deletion	UNP Q8CI75
B	?	-	SER	deletion	UNP Q8CI75
B	?	-	THR	deletion	UNP Q8CI75
B	?	-	PRO	deletion	UNP Q8CI75
B	?	-	VAL	deletion	UNP Q8CI75
B	?	-	MET	deletion	UNP Q8CI75
B	?	-	LYS	deletion	UNP Q8CI75
B	?	-	ASP	deletion	UNP Q8CI75
B	?	-	GLU	deletion	UNP Q8CI75
B	?	-	ASN	deletion	UNP Q8CI75
B	?	-	THR	deletion	UNP Q8CI75
B	?	-	PRO	deletion	UNP Q8CI75
B	?	-	ILE	deletion	UNP Q8CI75
B	?	-	PRO	deletion	UNP Q8CI75
B	?	-	GLN	deletion	UNP Q8CI75
B	?	-	ASP	deletion	UNP Q8CI75
B	?	-	THR	deletion	UNP Q8CI75
B	?	-	ARG	deletion	UNP Q8CI75
B	?	-	GLY	deletion	UNP Q8CI75
B	389	ASN	ASP	engineered mutation	UNP Q8CI75

- Molecule 2 is a RNA chain called U-U-U-U-U-U-U-U-U-U-U-U-U-U.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	14	Total	C	H	N	O	P	0	0	0
			421	126	141	28	112	14			
2	D	14	Total	C	H	N	O	P	0	0	0
			421	126	141	28	112	14			

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

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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	O 5	0	0
4	B	1	Total 1	O 1	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.
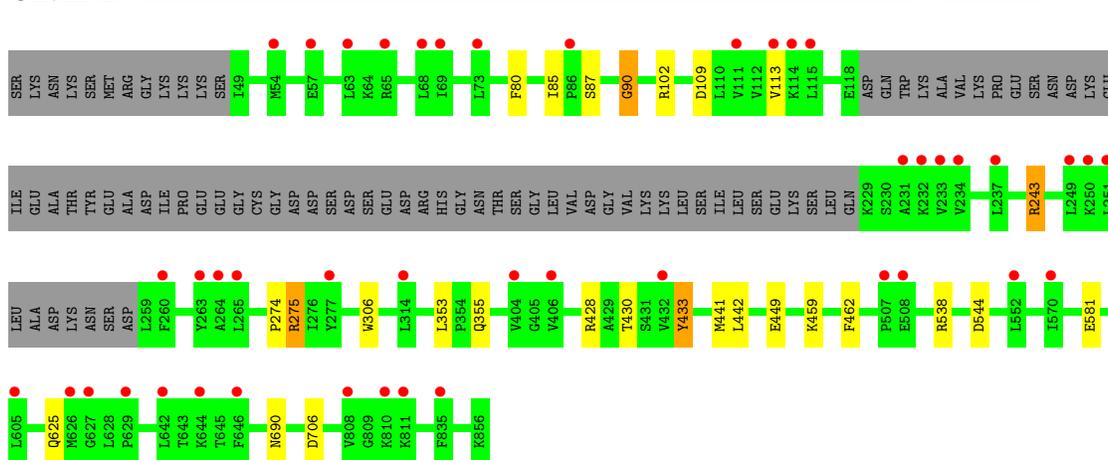
- Molecule 1: DIS3-like exonuclease 2

Chain A:
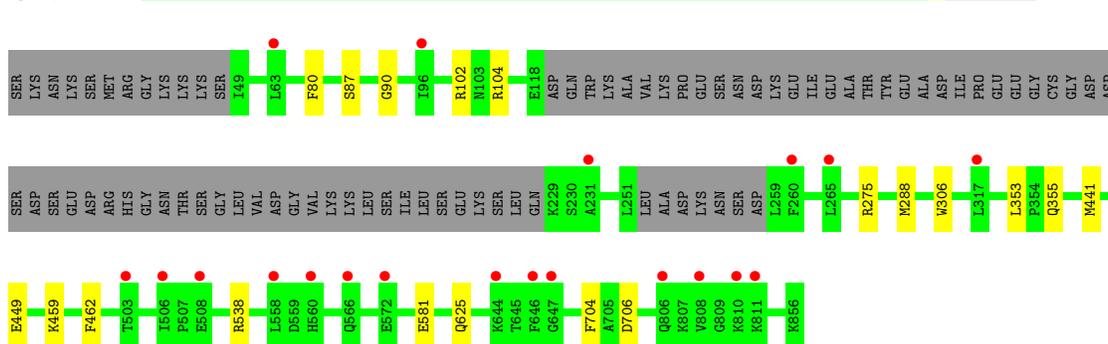
- Molecule 1: DIS3-like exonuclease 2

Chain B:

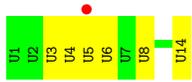- Molecule 2: U-U-U-U-U-U-U-U-U-U-U-U-U-U-U

Chain C:

- Molecule 2: U-U-U-U-U-U-U-U-U-U-U-U-U-U-U

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.93Å 96.08Å 157.31Å 90.00° 98.75° 90.00°	Depositor
Resolution (Å)	63.18 – 2.95 81.73 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.18-2.95) 99.8 (81.73-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.202 , 0.251 0.202 , 0.251	Depositor DCC
R_{free} test set	1999 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	60.0	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 33.4	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 39778 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22942	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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: 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	0.25	0/5624	0.40	0/7613
1	B	1.13	6/5624 (0.1%)	0.96	10/7613 (0.1%)
2	C	0.27	0/307	0.86	1/472 (0.2%)
2	D	0.27	0/307	0.73	0/472
All	All	0.80	6/11862 (0.1%)	0.74	11/16170 (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
1	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	433	TYR	CD2-CE2	50.24	2.14	1.39
1	B	433	TYR	CD1-CE1	49.86	2.14	1.39
1	B	433	TYR	CE1-CZ	-26.70	1.03	1.38
1	B	433	TYR	CE2-CZ	-25.27	1.05	1.38
1	B	433	TYR	CG-CD2	-16.26	1.18	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	433	TYR	CD1-CG-CD2	-34.08	80.41	117.90
1	B	433	TYR	CG-CD1-CE1	-30.13	97.20	121.30
1	B	433	TYR	CG-CD2-CE2	-28.78	98.27	121.30
1	B	433	TYR	CE1-CZ-CE2	-26.87	76.81	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	433	TYR	CB-CG-CD1	23.05	134.83	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	433	TYR	Sidechain

5.2 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 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	5508	5538	16	10	0
1	B	5508	5538	16	13	0
2	C	280	141	0	4	0
2	D	280	141	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
All	All	11584	11358	32	26	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 1.

The worst 5 of 26 close contacts within the same asymmetric unit are listed below:

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:ASP:OD2	1:B:243:ARG:NH2	2.29	0.66
1:A:80:PHE:O	1:A:102:ARG:NH2	2.32	0.63
1:A:625:GLN:OE1	1:A:625:GLN:N	2.33	0.62
1:A:449:GLU:O	1:A:459:LYS:NZ	2.33	0.61
1:B:80:PHE:O	1:B:102:ARG:NH2	2.32	0.61

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	685/770 (89%)	664 (97%)	21 (3%)	0	100	100
1	B	685/770 (89%)	662 (97%)	22 (3%)	1 (0%)	59	93
All	All	1370/1540 (89%)	1326 (97%)	43 (3%)	1 (0%)	59	93

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	GLY

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	613/682 (90%)	611 (100%)	2 (0%)	96	99
1	B	613/682 (90%)	609 (99%)	4 (1%)	91	98
All	All	1226/1364 (90%)	1220 (100%)	6 (0%)	94	99

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	243	ARG
1	B	706	ASP
1	B	275	ARG
1	A	706	ASP
1	B	462	PHE

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

such sidechains identified.

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	13/14 (92%)	7 (53%)	1 (7%)
2	D	13/14 (92%)	6 (46%)	0
All	All	26/28 (92%)	13 (50%)	1 (3%)

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	U
2	C	4	U
2	C	5	U
2	C	6	U
2	C	7	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	6	U

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.

5.7 Other polymers (i)

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	691/770 (89%)	0.60	20 (2%)	49	22	31, 62, 108, 156	0
1	B	691/770 (89%)	0.68	44 (6%)	19	10	41, 69, 123, 177	0
2	C	14/14 (100%)	0.69	1 (7%)	16	9	44, 99, 132, 163	0
2	D	14/14 (100%)	0.86	1 (7%)	16	9	52, 107, 145, 168	0
All	All	1410/1568 (89%)	0.64	66 (4%)	30	15	31, 65, 119, 177	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	646	PHE	10.4
1	B	646	PHE	9.2
1	A	260	PHE	5.5
1	A	644	LYS	5.0
1	B	65	ARG	4.7

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
3	MG	B	901	1/1	0.18	-0.96	51,51,51,51	0
3	MG	A	901	1/1	0.14	-2.22	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.