



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3N4Q
Title : Human cytomegalovirus terminase nuclease domain, Mn soaked
Authors : Nadal, M.; Mas, P.J.; Blanco, A.G.; Arnan, C.; Sola, M.; Hart, D.J.; Coll, M.
Deposited on : 2010-05-22
Resolution : 3.20 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

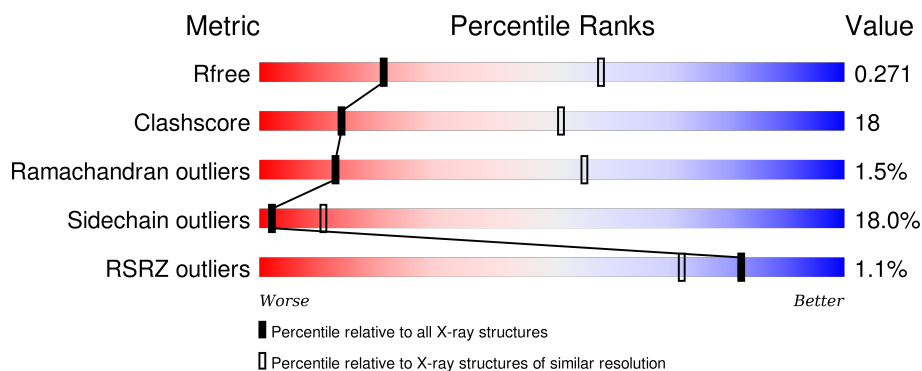
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	279	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>24%</div> <div>6%</div> <div>23%</div> </div> </div>
1	B	279	<div> <div></div> <div> <div>45%</div> <div>29%</div> <div>5%</div> <div>21%</div> </div> </div>
1	C	279	<div> <div>0%</div> <div> <div>45%</div> <div>25%</div> <div>7%</div> <div>22%</div> </div> </div>
1	D	279	<div> <div>0%</div> <div> <div>45%</div> <div>25%</div> <div>7%</div> <div>23%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7056 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 TERMINASE SUBUNIT UL89 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1736	1113	292	325	6			
1	B	221	Total	C	N	O	S	0	0	0
			1775	1137	301	331	6			
1	C	219	Total	C	N	O	S	0	0	0
			1755	1126	293	330	6			
1	D	214	Total	C	N	O	S	0	0	0
			1722	1104	290	322	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	MET	-	EXPRESSION TAG	UNP P16732
A	397	GLY	-	EXPRESSION TAG	UNP P16732
A	398	HIS	-	EXPRESSION TAG	UNP P16732
A	399	HIS	-	EXPRESSION TAG	UNP P16732
A	400	HIS	-	EXPRESSION TAG	UNP P16732
A	401	HIS	-	EXPRESSION TAG	UNP P16732
A	402	HIS	-	EXPRESSION TAG	UNP P16732
A	403	HIS	-	EXPRESSION TAG	UNP P16732
A	404	ASP	-	EXPRESSION TAG	UNP P16732
A	405	TYR	-	EXPRESSION TAG	UNP P16732
A	406	ASP	-	EXPRESSION TAG	UNP P16732
A	407	ILE	-	EXPRESSION TAG	UNP P16732
A	408	PRO	-	EXPRESSION TAG	UNP P16732
A	409	THR	-	EXPRESSION TAG	UNP P16732
A	410	THR	-	EXPRESSION TAG	UNP P16732
A	411	GLU	-	EXPRESSION TAG	UNP P16732
A	412	ASN	-	EXPRESSION TAG	UNP P16732
A	413	LEU	-	EXPRESSION TAG	UNP P16732
A	414	TYR	-	EXPRESSION TAG	UNP P16732
A	415	PHE	-	EXPRESSION TAG	UNP P16732
A	416	GLN	-	EXPRESSION TAG	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	-	EXPRESSION TAG	UNP P16732
B	396	MET	-	EXPRESSION TAG	UNP P16732
B	397	GLY	-	EXPRESSION TAG	UNP P16732
B	398	HIS	-	EXPRESSION TAG	UNP P16732
B	399	HIS	-	EXPRESSION TAG	UNP P16732
B	400	HIS	-	EXPRESSION TAG	UNP P16732
B	401	HIS	-	EXPRESSION TAG	UNP P16732
B	402	HIS	-	EXPRESSION TAG	UNP P16732
B	403	HIS	-	EXPRESSION TAG	UNP P16732
B	404	ASP	-	EXPRESSION TAG	UNP P16732
B	405	TYR	-	EXPRESSION TAG	UNP P16732
B	406	ASP	-	EXPRESSION TAG	UNP P16732
B	407	ILE	-	EXPRESSION TAG	UNP P16732
B	408	PRO	-	EXPRESSION TAG	UNP P16732
B	409	THR	-	EXPRESSION TAG	UNP P16732
B	410	THR	-	EXPRESSION TAG	UNP P16732
B	411	GLU	-	EXPRESSION TAG	UNP P16732
B	412	ASN	-	EXPRESSION TAG	UNP P16732
B	413	LEU	-	EXPRESSION TAG	UNP P16732
B	414	TYR	-	EXPRESSION TAG	UNP P16732
B	415	PHE	-	EXPRESSION TAG	UNP P16732
B	416	GLN	-	EXPRESSION TAG	UNP P16732
B	417	GLY	-	EXPRESSION TAG	UNP P16732
C	396	MET	-	EXPRESSION TAG	UNP P16732
C	397	GLY	-	EXPRESSION TAG	UNP P16732
C	398	HIS	-	EXPRESSION TAG	UNP P16732
C	399	HIS	-	EXPRESSION TAG	UNP P16732
C	400	HIS	-	EXPRESSION TAG	UNP P16732
C	401	HIS	-	EXPRESSION TAG	UNP P16732
C	402	HIS	-	EXPRESSION TAG	UNP P16732
C	403	HIS	-	EXPRESSION TAG	UNP P16732
C	404	ASP	-	EXPRESSION TAG	UNP P16732
C	405	TYR	-	EXPRESSION TAG	UNP P16732
C	406	ASP	-	EXPRESSION TAG	UNP P16732
C	407	ILE	-	EXPRESSION TAG	UNP P16732
C	408	PRO	-	EXPRESSION TAG	UNP P16732
C	409	THR	-	EXPRESSION TAG	UNP P16732
C	410	THR	-	EXPRESSION TAG	UNP P16732
C	411	GLU	-	EXPRESSION TAG	UNP P16732
C	412	ASN	-	EXPRESSION TAG	UNP P16732
C	413	LEU	-	EXPRESSION TAG	UNP P16732
C	414	TYR	-	EXPRESSION TAG	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	PHE	-	EXPRESSION TAG	UNP P16732
C	416	GLN	-	EXPRESSION TAG	UNP P16732
C	417	GLY	-	EXPRESSION TAG	UNP P16732
D	396	MET	-	EXPRESSION TAG	UNP P16732
D	397	GLY	-	EXPRESSION TAG	UNP P16732
D	398	HIS	-	EXPRESSION TAG	UNP P16732
D	399	HIS	-	EXPRESSION TAG	UNP P16732
D	400	HIS	-	EXPRESSION TAG	UNP P16732
D	401	HIS	-	EXPRESSION TAG	UNP P16732
D	402	HIS	-	EXPRESSION TAG	UNP P16732
D	403	HIS	-	EXPRESSION TAG	UNP P16732
D	404	ASP	-	EXPRESSION TAG	UNP P16732
D	405	TYR	-	EXPRESSION TAG	UNP P16732
D	406	ASP	-	EXPRESSION TAG	UNP P16732
D	407	ILE	-	EXPRESSION TAG	UNP P16732
D	408	PRO	-	EXPRESSION TAG	UNP P16732
D	409	THR	-	EXPRESSION TAG	UNP P16732
D	410	THR	-	EXPRESSION TAG	UNP P16732
D	411	GLU	-	EXPRESSION TAG	UNP P16732
D	412	ASN	-	EXPRESSION TAG	UNP P16732
D	413	LEU	-	EXPRESSION TAG	UNP P16732
D	414	TYR	-	EXPRESSION TAG	UNP P16732
D	415	PHE	-	EXPRESSION TAG	UNP P16732
D	416	GLN	-	EXPRESSION TAG	UNP P16732
D	417	GLY	-	EXPRESSION TAG	UNP P16732

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

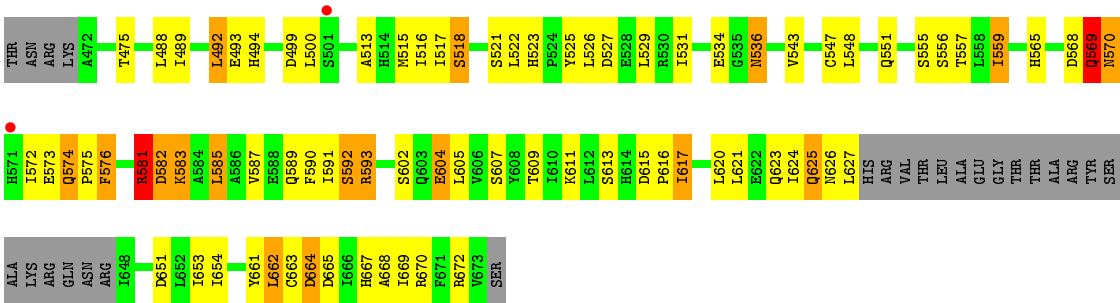
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0

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

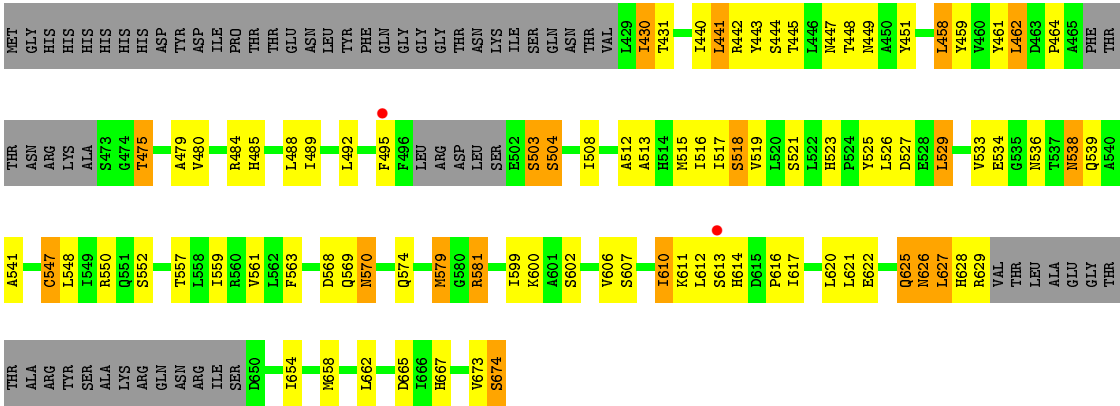
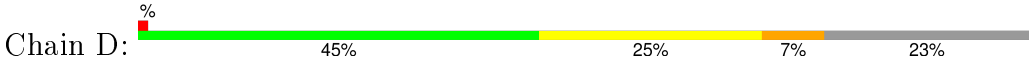
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	17	Total O 17 17	0	0
4	C	15	Total O 15 15	0	0
4	D	13	Total O 13 13	0	0



● Molecule 1: TERMINASE SUBUNIT UL89 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.70 Å 88.10 Å 190.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.05 – 3.20 44.05 – 3.19	Depositor EDS
% Data completeness (in resolution range)	89.6 (44.05-3.20) 89.6 (44.05-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.207 , 0.283 0.200 , 0.271	Depositor DCC
R_{free} test set	1108 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.820	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.6	EDS
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 21659 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7056	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: MG, 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	0.61	0/1770	0.75	1/2399 (0.0%)
1	B	0.58	1/1809 (0.1%)	0.74	2/2452 (0.1%)
1	C	0.58	0/1789	0.74	3/2427 (0.1%)
1	D	0.55	0/1756	0.69	0/2380
All	All	0.58	1/7124 (0.0%)	0.73	6/9658 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	622	GLU	CG-CD	5.10	1.59	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	LEU	CA-CB-CG	7.49	132.52	115.30
1	C	458	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	605	LEU	CA-CB-CG	5.69	128.38	115.30
1	C	569	GLN	N-CA-C	-5.46	96.27	111.00
1	B	578	LEU	CA-CB-CG	5.35	127.60	115.30

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	1736	0	1707	64	0
1	B	1775	0	1751	67	0
1	C	1755	0	1732	70	0
1	D	1722	0	1691	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	0	0	0
4	B	17	0	0	2	0
4	C	15	0	0	1	0
4	D	13	0	0	0	0
All	All	7056	0	6881	254	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 18.

The worst 5 of 254 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:B:664:ASP:HB2	4:B:18:HOH:O	1.55	1.03
1:D:464:PRO:HA	1:D:475:THR:HB	1.44	1.00
1:D:611:LYS:HB3	1:D:612:LEU:HD22	1.45	0.99
1:A:456:LYS:HD3	1:A:525:TYR:O	1.73	0.90
1:B:568:ASP:CG	1:B:569:GLN:H	1.77	0.87

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	208/279 (75%)	188 (90%)	15 (7%)	5 (2%)	7	43
1	B	213/279 (76%)	182 (85%)	29 (14%)	2 (1%)	21	67
1	C	213/279 (76%)	179 (84%)	30 (14%)	4 (2%)	10	50
1	D	206/279 (74%)	178 (86%)	26 (13%)	2 (1%)	19	65
All	All	840/1116 (75%)	727 (86%)	100 (12%)	13 (2%)	13	55

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	612	LEU
1	C	569	GLN
1	D	504	SER
1	A	537	THR
1	A	569	GLN

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	188/242 (78%)	154 (82%)	34 (18%)	2	11
1	B	192/242 (79%)	160 (83%)	32 (17%)	3	13
1	C	190/242 (78%)	154 (81%)	36 (19%)	2	10
1	D	186/242 (77%)	152 (82%)	34 (18%)	2	10
All	All	756/968 (78%)	620 (82%)	136 (18%)	2	11

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	663	CYS
1	C	529	LEU
1	D	579	MET
1	B	665	ASP
1	C	460	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	603	GLN
1	C	570	ASN
1	D	574	GLN
1	B	623	GLN
1	C	569	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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 [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 [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	216/279 (77%)	-0.32	5 (2%) 64 49	48, 77, 119, 164	6 (2%)
1	B	221/279 (79%)	-0.40	1 (0%) 91 87	53, 76, 110, 154	2 (0%)
1	C	219/279 (78%)	-0.32	2 (0%) 85 78	54, 82, 128, 180	4 (1%)
1	D	214/279 (76%)	-0.22	2 (0%) 85 78	57, 86, 122, 148	12 (5%)
All	All	870/1116 (77%)	-0.32	10 (1%) 82 72	48, 80, 123, 180	24 (2%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	612	LEU	3.3
1	D	613	SER	3.1
1	D	495	PHE	3.0
1	A	497	LEU	3.0
1	A	503	SER	2.8

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
2	MN	D	7	1/1	0.97	0.09	-2.27	60,60,60,60	0
3	MG	B	2	1/1	0.88	0.10	-2.59	40,40,40,40	0
2	MN	D	8	1/1	0.98	0.18	-	64,64,64,64	0
2	MN	C	6	1/1	0.98	0.06	-	58,58,58,58	0
2	MN	A	2	1/1	0.96	0.14	-	55,55,55,55	0
2	MN	B	3	1/1	0.98	0.05	-	55,55,55,55	0
3	MG	D	3	1/1	0.92	0.05	-	38,38,38,38	0
3	MG	A	675	1/1	0.95	0.08	-	29,29,29,29	0
2	MN	B	4	1/1	0.96	0.07	-	52,52,52,52	0
2	MN	A	1	1/1	0.96	0.12	-	58,58,58,58	0
3	MG	C	4	1/1	0.93	0.17	-	65,65,65,65	0
2	MN	C	5	1/1	0.96	0.07	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.