



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:00 PM GMT

PDB ID : 1N35
Title : lambda3 elongation complex with four phosphodiester bond formed
Authors : Tao, Y.; Farsetta, D.L.; Nibert, M.L.; Harrison, S.C.
Deposited on : 2002-10-25
Resolution : 2.50 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

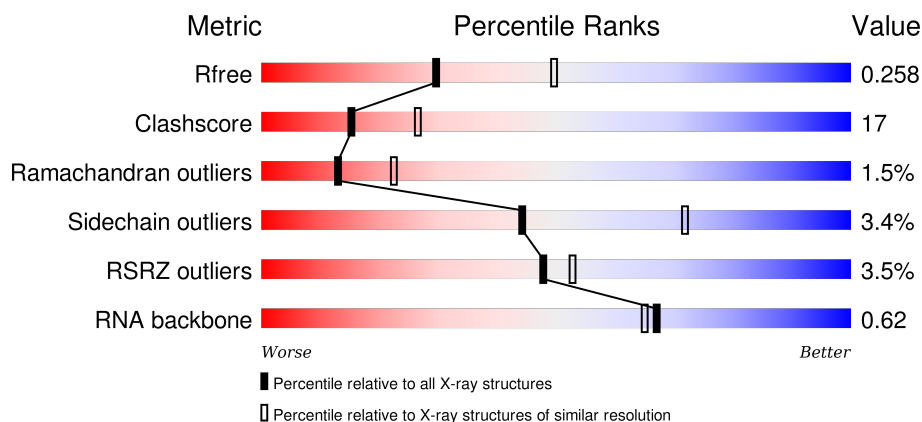
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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	B	5	<div> <div>100%</div> <div> <div>20%</div> <div>80%</div> </div> </div>
2	C	10	<div> <div>20%</div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
3	A	1267	<div> <div>3%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CH1	A	1294	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10703 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 RNA chain called 5'-R(P*GP*GP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	5	Total	C	N	O	P	0	0	0
			116	50	25	36	5			

- Molecule 2 is a RNA chain called 5'-R(*AP*UP*UP*AP*GP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			165	74	27	56	8			

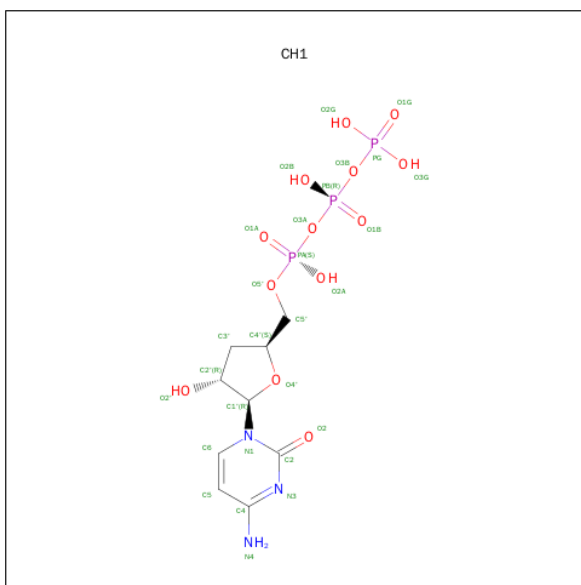
- Molecule 3 is a protein called Minor core protein lambda 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1264	Total	C	N	O	S	0	0	0
			9986	6369	1712	1841	64			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is 3'-DEOXY-CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CH1) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
5	A	1	Total 28	C 9	N 3	O 13	P 3	0	0

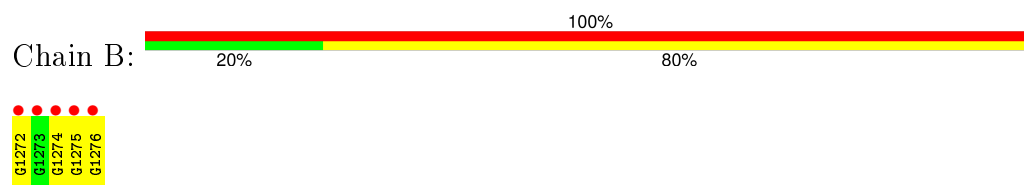
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	340	Total O 340 340	0	0
6	B	4	Total O 4 4	0	0
6	C	6	Total O 6 6	0	0

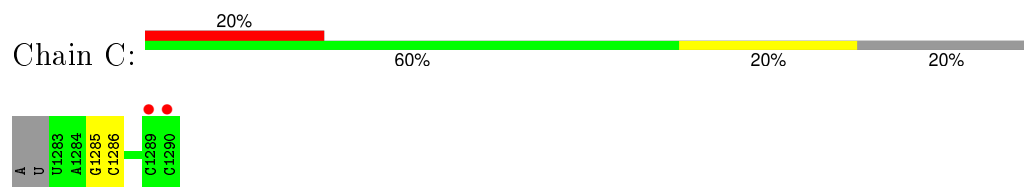
3 Residue-property plots

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.

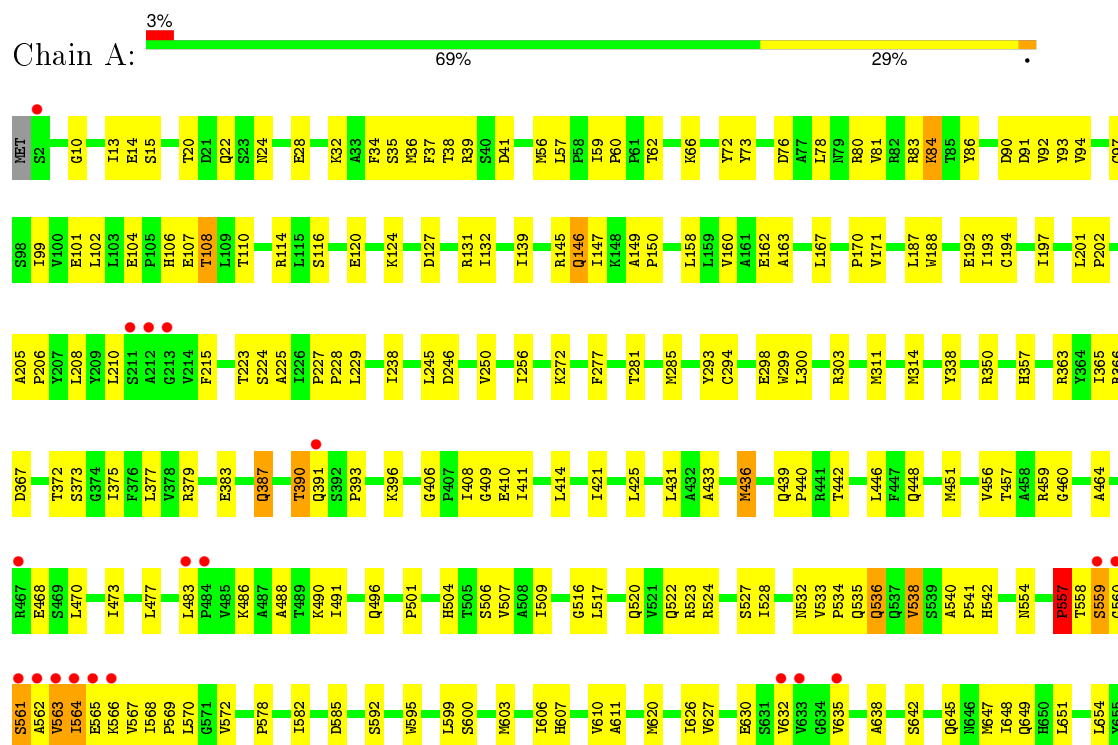
- Molecule 1: 5'-R(P*GP*GP*GP*GP*G)-3'



- Molecule 2: 5'-R(*AP*UP*UP*AP*GP*CP*CP*CP*CP*C)-3'



- Molecule 3: Minor core protein lambda 3



R1265	M1142	H1005	Q864	G777	K656
SER	D1120	P1006	L877	T778	F659
ALA	V1121	P1007	W878	A779	
	N1122	H1014	F881	E780	N671
	A1123	Q1018	W886	Y781	P681
	R1130	A1024	I887	L784	
	L1134	I1025	F888	Y785	T685
	G1135	A1026	S889	I787	A686
	A1136	E1029	W890	F788	T687
	L1146	M1034	T894	G789	E690
	G1149	A1040	R907	R791	
	L1150	R1041	P908	N794	M698
	Q1151	R1042	I909	L795	W706
	E1152	R1043	W920	S796	G707
	L1172	H1044	R923	R797	D712
	R1174	S1045	W926	F799	T724
	V1175	F1049	L940	E804	I725
	V1176	L1052	R941	R805	Q726
	P1181	L1053	Q944	W814	V730
	W1184	K1060	Q948	P815	C731
	M1185	W1061	P952	A816	
	L1199	R1062	R953	L817	D734
	L1200	M1063	R956	D819	D735
	P1201	C1064	R957	Q820	G742
	G1204	E1065	R960	I821	T743
	W1217	D1072	A961	W824	T744
	L1218	L1073	A962	V829	A745
	R1219	R1074	S963	Q834	G746
	R1223	D1082	R964	W835	K747
	A1237	P1083	R967	Q836	W748
	V1238	S1086	F968	R837	N749
	E1243	D1087	Y977	L845	S750
	H1246	P1088	L984	R851	E751
	F1256	L1090	R987	Q852	T752
	M1257	V1093	R990	M855	I753
	T1258	S1094	Q995	I856	Q754
	W1259	V1095	Q996	C857	N755
	M1260	Q1100	Q996	E858	D756
	R1261	S1101	I1002	S859	L757
	Q1262	T1102	I1003	W860	E758
	E1263	R1103	I1003	G861	L759
	G1264	F1106	H1004	Y862	I760

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.88Å 85.01Å 249.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.01 – 2.50 43.01 – 2.49	Depositor EDS
% Data completeness (in resolution range)	89.9 (43.01-2.50) 89.4 (43.01-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.259 0.207 , 0.258	Depositor DCC
R_{free} test set	2581 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53074 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10703	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CH1, 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	B	0.81	1/130 (0.8%)	0.68	0/201
2	C	0.52	0/182	0.71	0/280
3	A	0.38	0/10239	0.61	1/13905 (0.0%)
All	All	0.39	1/10551 (0.0%)	0.61	1/14386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1272	G	OP3-P	-7.10	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	408	ILE	N-CA-C	-5.48	96.19	111.00

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	B	116	0	56	8	0
2	C	165	0	88	4	0
3	A	9986	0	9903	354	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	84	0	36	3	0
6	A	340	0	0	8	0
6	B	4	0	0	0	0
6	C	6	0	0	0	0
All	All	10703	0	10083	356	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 17.

The worst 5 of 356 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)
3:A:223:THR:HG22	3:A:225:ALA:H	1.14	1.07
3:A:1112:MET:HE1	3:A:1150:LEU:HD11	1.33	1.05
3:A:410:GLU:H	3:A:649:GLN:NE2	1.58	1.01
1:B:1274:G:H21	3:A:562:ALA:HB2	1.22	1.01
3:A:81:VAL:H	3:A:671:ASN:HD21	1.09	0.99

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
3	A	1262/1267 (100%)	1169 (93%)	74 (6%)	19 (2%)	13 22

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	108	THR
3	A	559	SER

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Mol	Chain	Res	Type
3	A	561	SER
3	A	814	TRP
3	A	564	ILE

5.3.2 Protein sidechains [i](#)

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
3	A	1081/1083 (100%)	1044 (97%)	37 (3%)	44 72

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	735	ASP
3	A	804	GLU
3	A	1151	GLN
3	A	778	THR
3	A	784	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	664	ASN
3	A	710	HIS
3	A	1005	ASN
3	A	671	ASN
3	A	296	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	4/5 (80%)	0	0
2	C	7/10 (70%)	0	0
All	All	11/15 (73%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
5	CH1	A	1291	4	21,29,29	1.07	0	27,45,45	3.07	12 (44%)
5	CH1	A	1294	-	21,29,29	1.09	1 (4%)	27,45,45	3.02	11 (40%)
5	CH1	A	1295	-	21,29,29	1.10	1 (4%)	27,45,45	3.00	11 (40%)

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
5	CH1	A	1291	4	-	0/18/34/34	0/2/2/2
5	CH1	A	1294	-	-	0/18/34/34	0/2/2/2
5	CH1	A	1295	-	-	0/18/34/34	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1294	CH1	C6-N1	2.07	1.38	1.35
5	A	1295	CH1	C6-N1	2.22	1.38	1.35

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1295	CH1	O3G-PG-O1G	-9.28	80.69	110.58
5	A	1294	CH1	O3G-PG-O1G	-8.94	81.79	110.58
5	A	1291	CH1	O3G-PG-O1G	-8.90	81.95	110.58
5	A	1291	CH1	O3G-PG-O2G	-5.11	87.92	107.38
5	A	1295	CH1	O3G-PG-O2G	-5.07	88.09	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1291	CH1	2	0
5	A	1294	CH1	1	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	B	5/5 (100%)	4.61	5 (100%) 0 0	108, 119, 124, 124	0
2	C	8/10 (80%)	2.42	2 (25%) 1 1	35, 69, 127, 133	0
3	A	1264/1267 (99%)	0.02	38 (3%) 54 59	17, 32, 53, 98	0
All	All	1277/1282 (99%)	0.05	45 (3%) 48 53	17, 32, 54, 133	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1290	C	10.1
3	A	2	SER	8.3
3	A	561	SER	7.0
3	A	211	SER	6.9
2	C	1289	C	6.6

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
5	CH1	A	1294	28/28	0.65	0.33	2.19	86,99,118,119	0
5	CH1	A	1291	28/28	0.83	0.21	0.51	83,93,100,100	0
5	CH1	A	1295	28/28	0.88	0.20	-0.24	44,59,81,81	0
4	MN	A	1301	1/1	0.91	0.06	-4.55	63,63,63,63	0
4	MN	A	1302	1/1	0.98	0.11	-	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.