



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2026 – 06:05 PM EDT

PDB ID : 4I3H / pdb_00004i3h
Title : A three-gate structure of topoisomerase IV from *Streptococcus pneumoniae*
Authors : Ramaswamy, V.; Laponogov, I.; Veselkov, D.A.; Pan, X.S.; Crevel, I.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2012-11-26
Resolution : 3.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

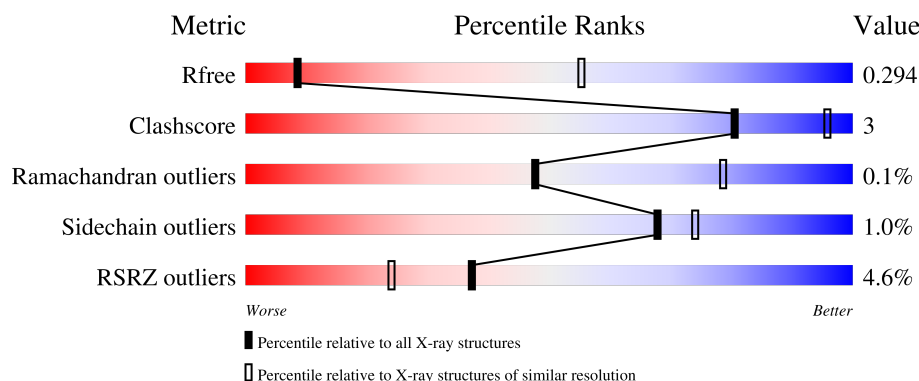
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

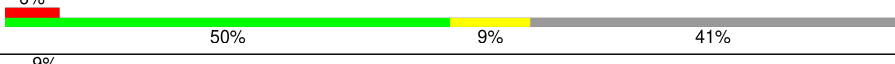
The reported resolution of this entry is 3.70 Å.

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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1144	
1	B	1144	
2	E	34	
2	G	34	
3	F	34	

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Mol	Chain	Length	Quality of chain
3	H	34	3% 56% 41%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30190 atoms, of which 13911 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 DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1037	Total	C	H	N	O	S	0	0	0
			14331	4753	6835	1290	1432	21			
1	B	1036	Total	C	H	N	O	S	0	0	0
			14018	4666	6625	1287	1418	22			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	ASP	ASN	conflict	UNP Q59961
A	460	ILE	VAL	conflict	UNP Q59961
A	996	ALA	THR	conflict	UNP Q59961
A	1000	HIS	-	linker	UNP Q59961
A	1257	THR	ILE	conflict	UNP P72525
A	1489	LEU	-	expression tag	UNP P72525
A	1490	GLU	-	expression tag	UNP P72525
A	1491	HIS	-	expression tag	UNP P72525
A	1492	HIS	-	expression tag	UNP P72525
A	1493	HIS	-	expression tag	UNP P72525
A	1494	HIS	-	expression tag	UNP P72525
A	1495	HIS	-	expression tag	UNP P72525
A	1496	HIS	-	expression tag	UNP P72525
B	217	ASP	ASN	conflict	UNP Q59961
B	460	ILE	VAL	conflict	UNP Q59961
B	996	ALA	THR	conflict	UNP Q59961
B	1000	HIS	-	linker	UNP Q59961
B	1257	THR	ILE	conflict	UNP P72525
B	1489	LEU	-	expression tag	UNP P72525
B	1490	GLU	-	expression tag	UNP P72525
B	1491	HIS	-	expression tag	UNP P72525
B	1492	HIS	-	expression tag	UNP P72525
B	1493	HIS	-	expression tag	UNP P72525
B	1494	HIS	-	expression tag	UNP P72525

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1495	HIS	-	expression tag	UNP P72525
B	1496	HIS	-	expression tag	UNP P72525

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*AP*AP*GP*GP*CP*GP*GP*TP*AP*AP*TP*AP*CP*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*AP*GP*AP*AP*TP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	20	Total	C	H	N	O	P	0	0	0
			637	196	225	77	119	20			
2	E	14	Total	C	N	O	P		0	0	0
			282	133	52	83	14				

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*CP*TP*GP*AP*TP*TP*CP*TP*GP*TP*GP*GP*AP*TP*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*CP*CP*GP*CP*CP*TP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	20	Total	C	H	N	O	P	0	0	0
			634	195	226	72	121	20			
3	F	14	Total	C	N	O	P		0	0	0
			283	133	51	85	14				

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

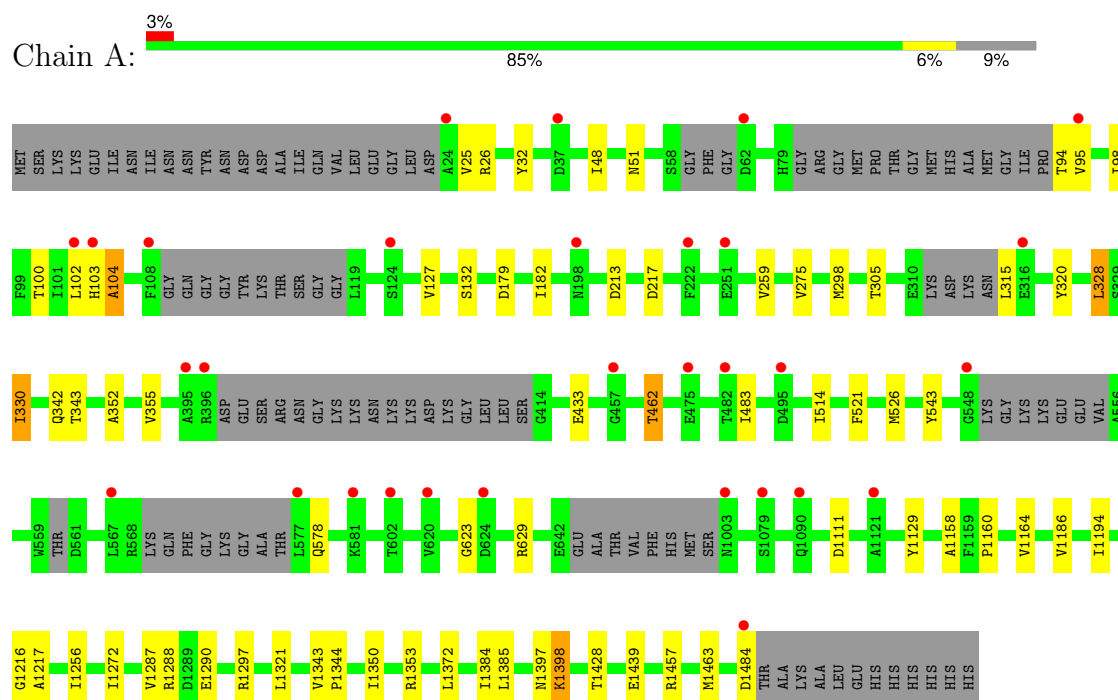
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	2	Total	O	0	0
			2	2		

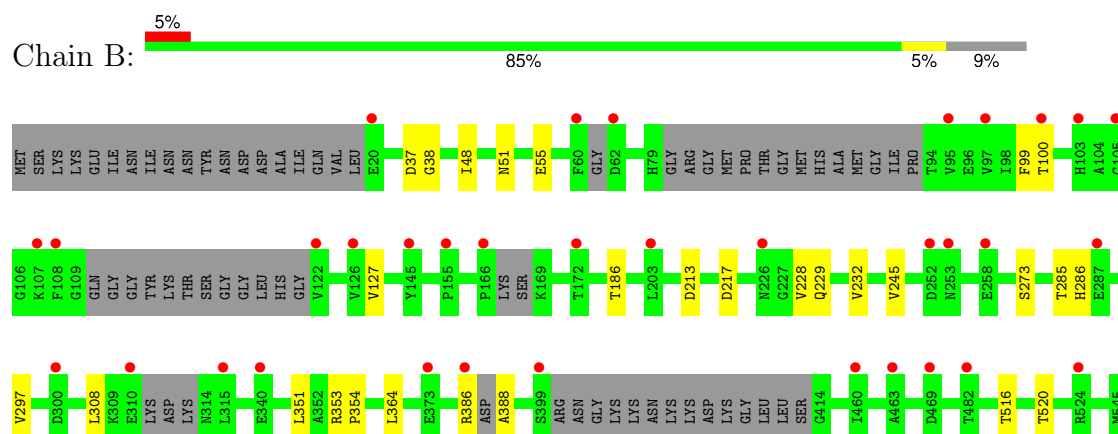
3 Residue-property plots [i](#)

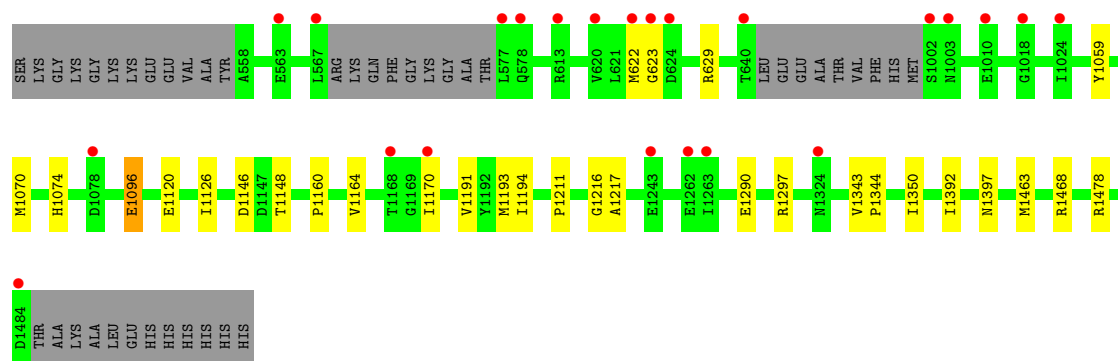
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A



- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A

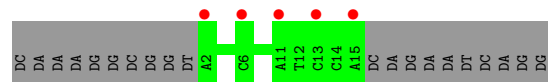




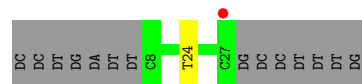
- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*GP*GP*CP*GP*GP*TP*AP*AP*TP*AP*CP*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*AP*GP*AP*AP*TP*CP*AP*GP*G)-3')



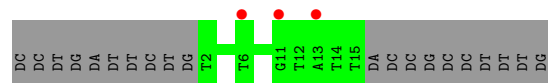
- Molecule 2: DNA (5'-D(*CP*AP*AP*AP*GP*GP*CP*GP*GP*TP*AP*AP*TP*AP*CP*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*AP*GP*AP*AP*TP*CP*AP*GP*G)-3')



- Molecule 3: DNA (5'-D(*CP*CP*TP*GP*AP*TP*TP*CP*TP*GP*TP*GP*GP*AP*TP*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*CP*CP*GP*CP*CP*TP*TP*TP*G)-3')



- Molecule 3: DNA (5'-D(*CP*CP*TP*GP*AP*TP*TP*CP*TP*GP*TP*GP*GP*AP*TP*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*CP*CP*GP*CP*CP*TP*TP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	160.60Å 160.60Å 280.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.82 – 3.70 71.82 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.82-3.70) 99.6 (71.82-3.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.10 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5058	Depositor
R, R_{free}	0.230 , 0.277 0.248 , 0.294	Depositor DCC
R_{free} test set	2006 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å ²)	95.5	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	30190	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: 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	0.13	0/7620	0.35	0/10384
1	B	0.13	0/7511	0.34	0/10237
2	E	0.29	0/316	0.59	0/483
2	G	0.24	0/462	0.63	0/711
3	F	0.28	0/317	0.56	0/485
3	H	0.24	0/456	0.68	0/701
All	All	0.14	0/16682	0.38	0/23001

There are no bond length outliers.

There are no bond angle outliers.

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	A	7496	6835	6823	41	0
1	B	7393	6625	6613	37	0
2	E	282	0	147	0	0
2	G	412	225	226	3	0
3	F	283	0	145	0	0
3	H	408	226	227	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	H	1	0	0	0	0
5	F	2	0	0	0	0
All	All	16279	13911	14181	79	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 3.

The worst 5 of 79 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:A:1288:ARG:NH1	1:A:1290:GLU:OE2	2.15	0.80
1:B:48:ILE:HG12	1:B:127:VAL:HG21	1.65	0.79
1:B:1191:VAL:HG11	1:B:1468:ARG:NH2	2.11	0.66
1:B:1194:ILE:HD11	1:B:1463:MET:HE2	1.79	0.64
1:B:1211:PRO:O	1:B:1478:ARG:NH2	2.30	0.64

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	1017/1144 (89%)	990 (97%)	25 (2%)	2 (0%)	43	72
1	B	1014/1144 (89%)	990 (98%)	24 (2%)	0	100	100
All	All	2031/2288 (89%)	1980 (98%)	49 (2%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ALA

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Mol	Chain	Res	Type
1	A	1398	LYS

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	
1	A	677/969 (70%)	668 (99%)	9 (1%)	61	71
1	B	648/969 (67%)	644 (99%)	4 (1%)	78	79
All	All	1325/1938 (68%)	1312 (99%)	13 (1%)	68	74

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1457	ARG
1	A	1484	ASP
1	B	1193	MET
1	B	308	LEU
1	B	1096	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	229	GLN
1	B	299	ASN
1	B	336	HIS
1	A	427	ASN
1	A	1006	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [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	1037/1144 (90%)	0.39	30 (2%) 53 33	39, 85, 130, 201	0
1	B	1036/1144 (90%)	0.48	57 (5%) 30 20	47, 92, 134, 183	0
2	E	14/34 (41%)	1.49	5 (35%) 1 1	77, 87, 91, 91	14 (100%)
2	G	20/34 (58%)	0.87	2 (10%) 12 13	67, 83, 150, 178	0
3	F	14/34 (41%)	1.32	3 (21%) 2 3	77, 87, 91, 92	14 (100%)
3	H	20/34 (58%)	0.88	1 (5%) 34 22	66, 87, 158, 185	0
All	All	2141/2424 (88%)	0.46	98 (4%) 37 24	39, 89, 132, 201	28 (1%)

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	ALA	3.9
1	B	1484	ASP	3.8
1	B	62	ASP	3.8
1	B	399	SER	3.6
1	B	300	ASP	3.6

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	1700	1/1	0.81	0.28	94,94,94,94	0
4	MG	H	1901	1/1	0.82	0.20	68,68,68,68	0
4	MG	B	1700	1/1	0.93	0.07	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.