



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:51 pm BST

PDB ID : 4N56
Title : Binary complex structure of Klenow fragment of Taq DNA polymerase I707L mutant (Cs3C KlenTaq) with DNA
Authors : Wu, E.Y.
Deposited on : 2013-10-09
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

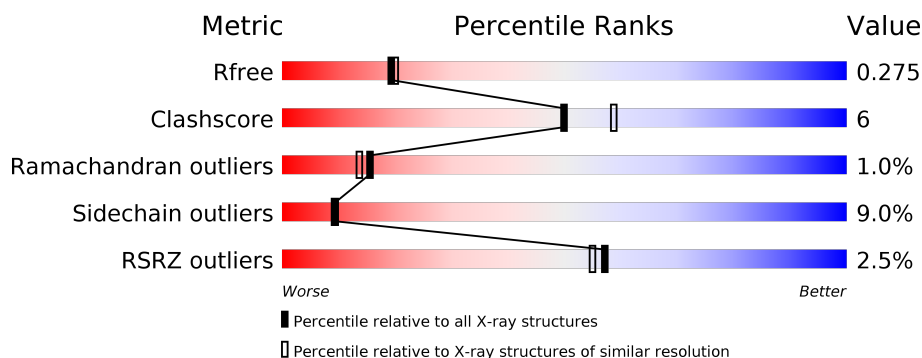
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	B	12	<div> <div style="width: 83%;"></div> <div style="width: 17%;"></div> </div> <div>83% 17%</div>
2	C	16	<div> <div style="width: 50%;"></div> <div style="width: 31%;"></div> <div style="width: 13%;"></div> <div style="width: 6%;"></div> </div> <div>50% 31% 13% 6%</div>
3	A	553	<div> <div style="width: 2%;"></div> <div style="width: 73%;"></div> <div style="width: 14%;"></div> <div style="width: 11%;"></div> </div> <div>2% 73% 14% 11%</div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4431 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 DNA chain called 5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*(D OC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			240	114	48	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			312	146	61	90	15			

- Molecule 3 is a protein called DNA polymerase I, thermostable.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	494	Total	C	N	O	S	0	0	0
			3850	2448	694	698	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	MET	-	INITIATING METHIONINE	UNP P19821
A	707	LEU	ILE	ENGINEERED MUTATION	UNP P19821

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mn	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is water.

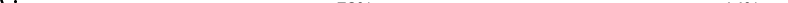
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	4	Total	O	0	0
			4	4		
7	C	5	Total	O	0	0
			5	5		
7	A	12	Total	O	0	0
			12	12		

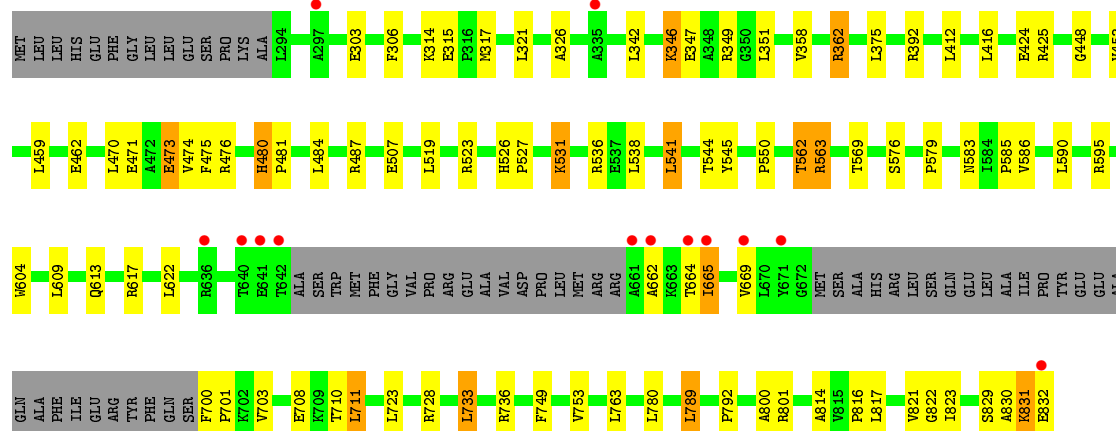
- Molecule 1: 5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*CP*(DOC))-3'



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



- Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.04 Å 110.04 Å 91.29 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.65 – 2.20 47.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.65-2.20) 98.6 (47.65-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.223 , 0.273 0.226 , 0.275	Depositor DCC
R_{free} test set	1615 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4431	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, MN, DOC

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	0.61	0/249	0.91	0/382
2	C	0.71	0/350	0.98	2/539 (0.4%)
3	A	0.68	0/3927	0.89	7/5325 (0.1%)
All	All	0.68	0/4526	0.90	9/6246 (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
3	A	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	214	DG	C1'-O4'-C4'	-6.48	103.62	110.10
3	A	563	ARG	CG-CD-NE	6.20	124.82	111.80
3	A	728	ARG	NE-CZ-NH1	5.93	123.27	120.30
3	A	728	ARG	NE-CZ-NH2	-5.74	117.43	120.30
3	A	536	ARG	NE-CZ-NH1	5.71	123.16	120.30
3	A	349	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	C	204	DG	P-O3'-C3'	5.22	125.97	119.70
3	A	789	LEU	CA-CB-CG	5.18	127.20	115.30
3	A	733	LEU	CB-CG-CD1	5.06	119.61	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	831	LYS	Peptide

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	B	240	0	134	2	0
2	C	312	0	168	6	0
3	A	3850	0	3870	42	0
4	C	1	0	0	0	0
5	A	6	0	8	1	0
6	A	1	0	0	0	0
7	A	12	0	0	0	0
7	B	4	0	0	0	0
7	C	5	0	0	0	0
All	All	4431	0	4180	50	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 6.

All (50) 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:C:204:DG:H4'	2:C:205:DG:OP2	1.74	0.86
3:A:474:VAL:HG21	3:A:484:LEU:HD11	1.58	0.86
3:A:562:THR:HG21	3:A:576:SER:OG	1.78	0.83
3:A:562:THR:HG23	3:A:579:PRO:O	1.77	0.83
3:A:317:MET:HE1	3:A:362:ARG:HB3	1.74	0.69
3:A:562:THR:CG2	3:A:579:PRO:O	2.43	0.65
3:A:723:LEU:HD23	3:A:723:LEU:C	2.16	0.64
3:A:562:THR:HG21	3:A:576:SER:HG	1.59	0.64
3:A:800:ALA:HB1	3:A:821:VAL:HG11	1.81	0.63
3:A:723:LEU:O	3:A:723:LEU:HD23	1.99	0.62
3:A:662:ALA:O	3:A:665:ILE:HG22	2.00	0.62
3:A:317:MET:HE3	3:A:358:VAL:HG13	1.82	0.62
3:A:473:GLU:OE1	3:A:476:ARG:NH2	2.36	0.58
3:A:317:MET:CE	3:A:362:ARG:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:471:GLU:HG2	3:A:475:PHE:CE2	2.39	0.57
3:A:711:LEU:HD11	3:A:749:PHE:CE2	2.41	0.55
3:A:470:LEU:O	3:A:474:VAL:HG13	2.06	0.55
2:C:203:DA:H2''	2:C:205:DG:O6	2.07	0.54
3:A:617:ARG:NH1	3:A:816:PRO:O	2.42	0.52
3:A:711:LEU:CD1	3:A:749:PHE:CE2	2.93	0.52
3:A:604:TRP:CZ3	3:A:792:PRO:HD3	2.45	0.52
3:A:474:VAL:HG12	3:A:531:LYS:HB3	1.92	0.51
3:A:351:LEU:HD11	3:A:412:LEU:HD12	1.92	0.51
3:A:317:MET:HE3	3:A:358:VAL:CG1	2.43	0.49
2:C:210:DC:H2'	2:C:211:DG:C8	2.48	0.49
3:A:346:LYS:HD2	3:A:347:GLU:H	1.78	0.48
3:A:425:ARG:NH2	3:A:723:LEU:O	2.46	0.48
2:C:214:DG:C8	2:C:215:DT:H72	2.48	0.48
3:A:544:THR:O	5:A:901:GOL:H31	2.13	0.47
3:A:595:ARG:NH1	3:A:832:GLU:OXT	2.46	0.47
3:A:474:VAL:CG2	3:A:484:LEU:HD11	2.39	0.47
3:A:306:PHE:O	3:A:326:ALA:HA	2.15	0.46
2:C:214:DG:H2''	2:C:215:DT:O5'	2.15	0.46
3:A:609:LEU:CD2	3:A:821:VAL:HG13	2.47	0.45
3:A:541:LEU:HD23	3:A:590:LEU:HD23	1.97	0.45
3:A:448:GLY:O	3:A:780:LEU:HD22	2.17	0.44
3:A:545:TYR:CE1	3:A:585:PRO:HD3	2.54	0.43
3:A:700:PHE:N	3:A:701:PRO:HD3	2.34	0.43
3:A:453:VAL:HG13	3:A:550:PRO:HB3	2.01	0.43
2:C:204:DG:C4'	2:C:205:DG:OP2	2.58	0.42
3:A:723:LEU:CD2	3:A:723:LEU:C	2.87	0.42
3:A:526:HIS:ND1	3:A:527:PRO:HD2	2.35	0.42
3:A:822:GLY:O	3:A:823:ILE:HG13	2.20	0.42
3:A:669:VAL:CG1	3:A:703:VAL:HG11	2.50	0.41
3:A:315:GLU:HA	3:A:563:ARG:HD2	2.03	0.41
3:A:480:HIS:HA	3:A:481:PRO:HD3	1.92	0.41
1:B:111:DC:H2'	1:B:112:DOC:C6	2.50	0.41
3:A:664:THR:HG22	3:A:664:THR:O	2.21	0.40
1:B:112:DOC:O5'	1:B:112:DOC:H6	2.21	0.40
3:A:829:SER:O	3:A:830:ALA:C	2.60	0.40

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	488/553 (88%)	465 (95%)	18 (4%)	5 (1%)	15 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	831	LYS
3	A	814	ALA
3	A	613	GLN
3	A	586	VAL
3	A	665	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	388/453 (86%)	353 (91%)	35 (9%)	9 9

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	303	GLU
3	A	314	LYS
3	A	321	LEU
3	A	342	LEU
3	A	346	LYS
3	A	362	ARG

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Mol	Chain	Res	Type
3	A	375	LEU
3	A	392	ARG
3	A	416	LEU
3	A	424	GLU
3	A	459	LEU
3	A	462	GLU
3	A	473	GLU
3	A	480	HIS
3	A	487	ARG
3	A	507	GLU
3	A	519	LEU
3	A	523	ARG
3	A	531	LYS
3	A	538	LEU
3	A	541	LEU
3	A	562	THR
3	A	569	THR
3	A	583	ASN
3	A	622	LEU
3	A	708	GLU
3	A	710	THR
3	A	711	LEU
3	A	733	LEU
3	A	736	ARG
3	A	753	VAL
3	A	763	LEU
3	A	789	LEU
3	A	801	ARG
3	A	817	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	333	HIS
3	A	443	HIS
3	A	565	ASN
3	A	583	ASN
3	A	666	ASN
3	A	754	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	DOC	B	112	1,2	14,19,20	0.96	0	13,26,29	1.71	3 (23%)

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
1	DOC	B	112	1,2	-	0/4/18/19	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	DOC	C2-N3-C4	3.90	120.30	116.34
1	B	112	DOC	O4'-C1'-C2'	2.67	109.56	106.67
1	B	112	DOC	O4'-C4'-C5'	2.55	113.71	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	112	DOC	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	GOL	A	901	-	5,5,5	0.27	0	5,5,5	0.63	0

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	GOL	A	901	-	-	0/4/4/4	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	GOL	1	0

5.7 Other polymers

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	B	11/12 (91%)	-0.46	0 100 100	35, 40, 61, 63	0
2	C	15/16 (93%)	-0.23	0 100 100	37, 42, 86, 88	0
3	A	494/553 (89%)	0.14	13 (2%) 56 53	34, 53, 84, 106	0
All	All	520/581 (89%)	0.11	13 (2%) 57 55	34, 53, 84, 106	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	661	ALA	6.7
3	A	671	TYR	6.4
3	A	642	THR	5.3
3	A	664	THR	4.7
3	A	640	THR	4.6
3	A	636	ARG	3.4
3	A	669	VAL	3.3
3	A	641	GLU	3.3
3	A	662	ALA	3.3
3	A	335	ALA	2.7
3	A	832	GLU	2.7
3	A	297	ALA	2.7
3	A	665	ILE	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	DOC	B	112	18/19	0.97	0.12	33,40,47,48	0

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. 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(\AA^2)	Q<0.9
6	MG	A	902	1/1	0.78	0.19	59,59,59,59	0
5	GOL	A	901	6/6	0.95	0.18	39,40,41,43	0
4	MN	C	301	1/1	0.97	0.17	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.