



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:17 AM UTC

PDB ID : 4AQU / pdb_00004aqu
Title : Crystal structure of I-CreI complexed with its target methylated at position plus 2 (in the b strand) in the presence of calcium
Authors : Valton, J.; Daboussi, F.; Leduc, S.; Redondo, P.; Macmaster, R.; Molina, R.; Montoya, G.; Duchateau, P.
Deposited on : 2012-04-19
Resolution : 2.30 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 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

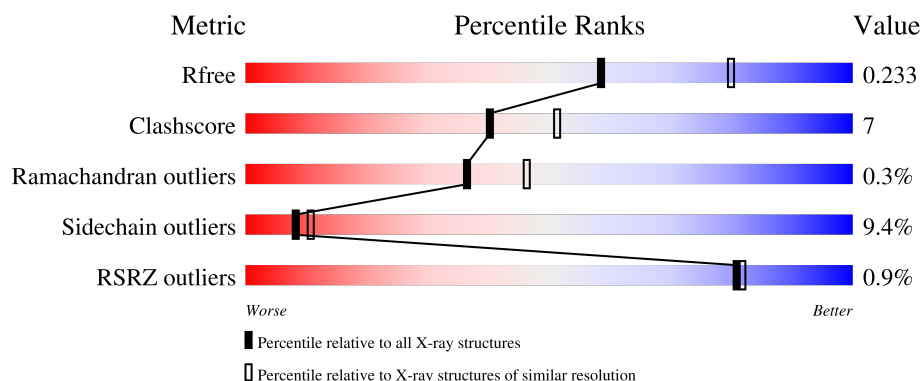
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	152	% 81% 16% .
1	B	152	% 79% 17% ..
2	C	24	67% 29% .
3	D	24	75% 17% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3567 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 DNA ENDONUCLEASE I-CREI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1236	796	210	229	1			
1	B	152	Total	C	N	O	S	0	0	0
			1236	796	210	229	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	24	Total	C	N	O	P	1	0	0
			494	236	94	141	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	24	Total	C	N	O	P	0	0	0
			485	234	85	143	23			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

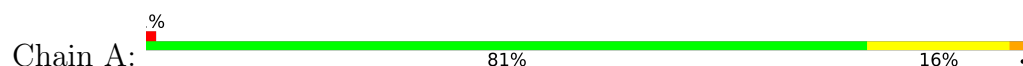
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total	O	0	0
			52	52		
6	B	23	Total	O	0	0
			23	23		
6	C	18	Total	O	0	0
			18	18		
6	D	9	Total	O	0	0
			9	9		

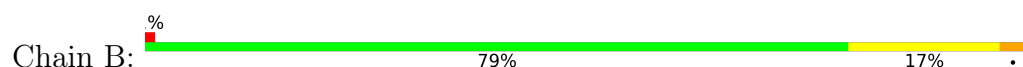
3 Residue-property plots [i](#)

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 ENDONUCLEASE I-CREI



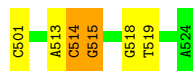
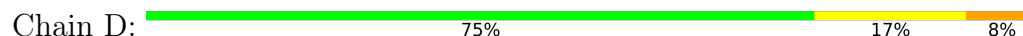
- Molecule 1: DNA ENDONUCLEASE I-CREI



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



- Molecule 3: 5'-D(*DCP*CP*AP*AP*AP*CP*TP*GP*TP*CP*TP*CP*AP*5CMP *GP*AP*CP*GP*TP*TP*TP*TP*GP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	71.58Å 45.35Å 172.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.80 – 2.30 44.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.80-2.30) 99.7 (44.80-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.196 , 0.249 0.184 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (7.77%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3567	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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, CA, 5CM

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	0.47	0/1259	0.75	0/1700
1	B	0.48	0/1259	0.77	1/1700 (0.1%)
2	C	0.34	0/555	0.99	1/856 (0.1%)
3	D	0.33	0/519	0.98	1/796 (0.1%)
All	All	0.44	0/3592	0.84	3/5052 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	THR	N-CA-C	-5.65	105.27	111.82
2	C	414	DA	N9-C1'-C2'	5.40	121.60	113.50
3	D	515	DG	P-O5'-C5'	5.22	127.83	120.00

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	1236	0	1270	20	0
1	B	1236	0	1270	15	0
2	C	494	0	272	8	0
3	D	485	0	275	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	52	0	0	3	0
6	B	23	0	0	0	0
6	C	18	0	0	0	0
6	D	9	0	0	0	0
All	All	3567	0	3103	43	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 7.

All (43) 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:324:GLU:O	1:B:327:THR:HG22	1.84	0.78
1:A:123:LEU:HD21	1:A:149:ARG:HG2	1.72	0.71
1:B:281:ILE:HG23	1:B:282:LYS:HG3	1.74	0.68
3:D:518:DG:H2''	3:D:519:DT:H5'	1.79	0.64
1:A:62:ILE:HG22	1:A:64:VAL:HG12	1.83	0.60
1:A:52:ARG:NH1	1:A:69:ASP:OD1	2.35	0.60
1:A:151:VAL:C	1:A:153:ASP:H	2.10	0.59
6:A:2003:HOH:O	3:D:515:DG:OP2	2.17	0.58
2:C:401:DT:H2''	2:C:402:DC:H5''	1.88	0.56
2:C:418:DA:H2''	2:C:419:DG:H5'	1.88	0.55
1:B:330:ASP:OD1	1:B:341:ARG:NH2	2.40	0.54
1:B:228:LYS:NZ	2:C:419:DG:O6	2.34	0.51
1:A:124:GLU:O	1:A:127:THR:HB	2.12	0.49
1:B:235:PHE:HE2	1:B:316:LYS:HA	1.78	0.48
1:B:344:THR:H	1:B:347:THR:HG23	1.78	0.48
1:B:312:LEU:N	1:B:313:PRO:CD	2.78	0.46
1:B:318:SER:OG	1:B:321:LYS:N	2.38	0.46
1:A:142:LYS:HG3	3:D:518:DG:H5''	1.99	0.45
1:B:292:GLN:HE21	1:B:292:GLN:HB3	1.63	0.45
2:C:418:DA:H2''	2:C:419:DG:C5'	2.46	0.45
1:A:123:LEU:HD21	1:A:149:ARG:CG	2.43	0.44
1:A:130:ASP:OD1	1:A:141:ARG:NH2	2.48	0.44
1:A:130:ASP:HA	1:A:141:ARG:NH2	2.32	0.43
1:A:151:VAL:C	1:A:153:ASP:N	2.74	0.43
6:A:2052:HOH:O	2:C:415:DG:H5'	2.18	0.43
1:B:232:SER:O	3:D:501:DC:H2'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LYS:HE3	1:B:324:GLU:OE1	2.19	0.43
2:C:413:DG:H1'	2:C:414:DA:O4'	2.19	0.42
1:A:82:LYS:HB2	1:A:83:PRO:HD3	2.00	0.42
2:C:402:DC:H2''	2:C:403:DA:H5'	2.01	0.42
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.72	0.42
1:B:302:ALA:O	1:B:306:LEU:HB2	2.19	0.42
1:A:22:SER:HB3	1:A:44:GLN:HG2	2.02	0.42
1:A:73:VAL:HG21	3:D:514:5CM:H5A1	2.01	0.42
1:A:141:ARG:NH1	6:A:2008:HOH:O	2.34	0.42
1:A:33:TYR:OH	2:C:403:DA:N7	2.51	0.41
1:B:228:LYS:HA	1:B:229:PRO:HD2	1.83	0.41
1:A:54:PHE:CD2	1:B:297:LEU:HD21	2.56	0.41
1:A:28:LYS:O	1:A:37:HIS:HA	2.21	0.40
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.95	0.40
1:A:127:THR:O	1:A:130:ASP:HB2	2.22	0.40
1:B:344:THR:C	1:B:346:GLU:H	2.29	0.40
3:D:513:DA:H1'	3:D:514:5CM:O4'	2.22	0.40

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	150/152 (99%)	143 (95%)	6 (4%)	1 (1%)	18	23
1	B	150/152 (99%)	137 (91%)	13 (9%)	0	100	100
All	All	300/304 (99%)	280 (93%)	19 (6%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	LEU

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	139/139 (100%)	129 (93%)	10 (7%)	13	18
1	B	139/139 (100%)	123 (88%)	16 (12%)	5	6
All	All	278/278 (100%)	252 (91%)	26 (9%)	8	11

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	41	LEU
1	A	73	VAL
1	A	81	ILE
1	A	118	SER
1	A	121	LYS
1	A	123	LEU
1	A	124	GLU
1	A	127	THR
1	A	141	ARG
1	B	203	THR
1	B	204	LYS
1	B	257	LYS
1	B	269	ASP
1	B	273	VAL
1	B	281	ILE
1	B	307	LYS
1	B	314	SER
1	B	316	LYS
1	B	317	GLU
1	B	318	SER
1	B	321	LYS
1	B	329	VAL
1	B	344	THR
1	B	347	THR
1	B	349	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	237	HIS
1	B	244	GLN
1	B	331	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
3	5CM	D	514	3,2,4	18,21,22	3.34	8 (44%)	24,30,33	2.95	7 (29%)

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
3	5CM	D	514	3,2,4	-	1/7/21/22	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	514	5CM	C6-C5	8.63	1.48	1.34
3	D	514	5CM	C4-N3	4.99	1.42	1.34
3	D	514	5CM	C5-C4	4.87	1.47	1.44
3	D	514	5CM	C2-N3	4.85	1.46	1.36
3	D	514	5CM	C6-N1	4.06	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	514	5CM	C4-N4	3.99	1.44	1.34
3	D	514	5CM	C2-N1	2.66	1.45	1.40
3	D	514	5CM	C3'-C4'	-2.42	1.46	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	514	5CM	C1'-N1-C2	9.01	133.29	117.83
3	D	514	5CM	C1'-N1-C6	-7.60	107.98	120.74
3	D	514	5CM	C2'-C1'-N1	4.31	124.58	113.81
3	D	514	5CM	C5-C6-N1	-3.74	119.25	123.31
3	D	514	5CM	O4'-C1'-N1	3.54	114.16	107.86
3	D	514	5CM	C5-C4-N3	-2.34	119.36	121.75
3	D	514	5CM	N1-C2-N3	2.05	122.36	118.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	514	5CM	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	514	5CM	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	1354	-	5,5,5	0.41	0	5,5,5	0.40	0
5	GOL	A	1155	-	5,5,5	0.41	0	5,5,5	0.27	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	B	1354	-	-	0/4/4/4	-
5	GOL	A	1155	-	-	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.

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	152/152 (100%)	-0.29	1 (0%) 84 85	19, 36, 65, 84	0
1	B	152/152 (100%)	0.00	2 (1%) 75 76	21, 44, 79, 99	0
2	C	24/24 (100%)	-0.90	0 100 100	26, 36, 51, 57	0
3	D	23/24 (95%)	-0.88	0 100 100	24, 37, 47, 54	0
All	All	351/352 (99%)	-0.24	3 (0%) 81 82	19, 38, 75, 99	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	ASP	4.1
1	A	153	ASP	2.8
1	B	250	GLN	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(Å ²)	Q<0.9
3	5CM	D	514	20/21	0.98	0.06	19,30,38,47	0

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
5	GOL	A	1155	6/6	0.94	0.12	44,52,55,56	0
5	GOL	B	1354	6/6	0.94	0.12	48,53,56,56	0
4	CA	A	1154	1/1	0.99	0.02	22,22,22,22	0
4	CA	A	1156	1/1	0.99	0.01	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.