W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:43 AM GMT

PDB ID	:	2ICE
Title	:	CRIg bound to C3c
Authors	:	Wiesmann, C.
Deposited on	:	2006-09-12
Resolution	:	3.10 Å(reported)

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

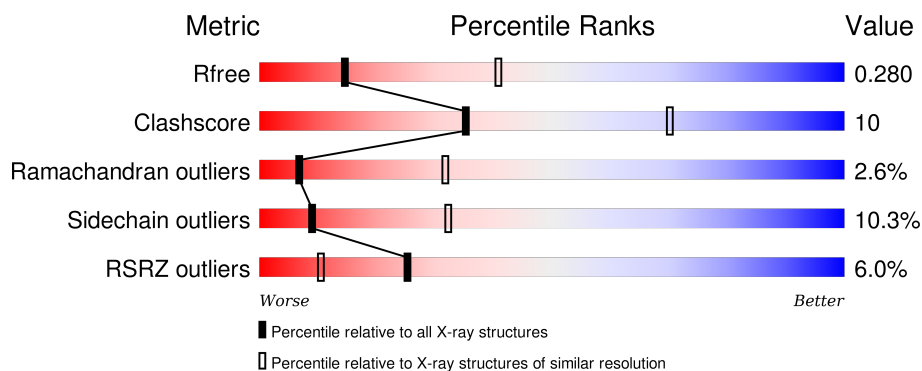|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 <=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	642	% 70% 25% 5%
1	D	642	6% 70% 25% • •
2	B	206	63% 24% • 11%
2	E	206	% 58% 29% • 11%
3	C	343	3% 56% 26% • • 14%

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	343	27% / 64% / 19% / 14%
4	S	119	% / 72% / 26%
4	T	119	2% / 73% / 24%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19619 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total 5008	C 3188	N 848	O 957	S 15	0	0	0
1	D	630	Total 4907	C 3127	N 828	O 937	S 15	0	0	0

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total 1480	C 950	N 249	O 276	S 5	0	0	0
2	E	183	Total 1480	C 950	N 249	O 276	S 5	0	0	0

- Molecule 3 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	296	Total 2407	C 1517	N 395	O 475	S 20	0	0	0
3	F	296	Total 2407	C 1517	N 395	O 475	S 20	0	0	0

- Molecule 4 is a protein called V-set and immunoglobulin domain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S	119	Total 950	C 595	N 169	O 183	S 3	0	0	0
4	T	119	Total 950	C 595	N 169	O 183	S 3	0	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Ca 1	0	0
6	D	1	Total 1	Ca 1	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: Complement C3 beta chain

- Molecule 1: Complement C3 beta chain

E442 L443 R444 T448 L449 N452 F453 K464 T469 I472 E487 L478 L479 K480 E487 Q490 D491 L492 V493 I499 R508 L509 V510 A511 Y512 Y513 T514 L515 A518 S519 Q520 Q521 R522 S528 V529 W530 V531 D532 V533 K534 V538 G539 S545 G546 Q547 S548

E549 D550 N551 Q552 P553 V554 P555 Q558 M559 T560 L561 K562 D566 H567 K578 L583 N584 N587 T590 K593 I594 T606 P607 G608 S609 G610 K611 S618 F624 T625 S628 G629 Q630 Q631 R635 A636 E637 L638 Q639 C640 P641 Q642

• Molecule 2: Complement C3 alpha chain

Chain B:

63%　24%　11%

SER ASN LEU D730 E731 I734 A735 N738 S741 R742 S743 E744 F745 P746 E747 S748 W751 N752 V753 K767 I771 F772 L773 L774 D775 D779 W780 M787 S788 D789 K790 K791 A796 E800 L811 R812 L813 Y830 N831 Y832 N835 L838 R841

N847 P848 C851 S852 L853 A854 H860 S870 S871 L872 V877 I878 K882 T883 V888 E889 V890 V894 H897 S900 V909 E912 GLY ILE ARG MET ASN LYS THR VAL ALA VAL ARG THR LEU ASP PRO GLU ARG LEU GLY ARG

• Molecule 2: Complement C3 alpha chain

Chain E:

%
58%　29%　11%

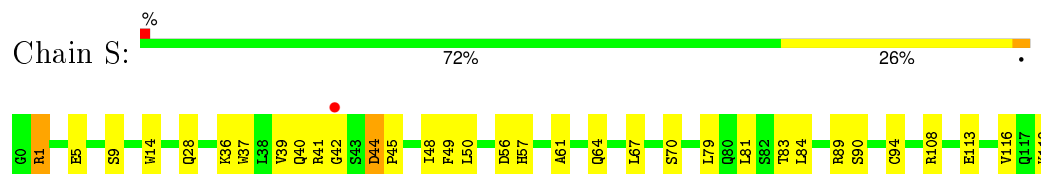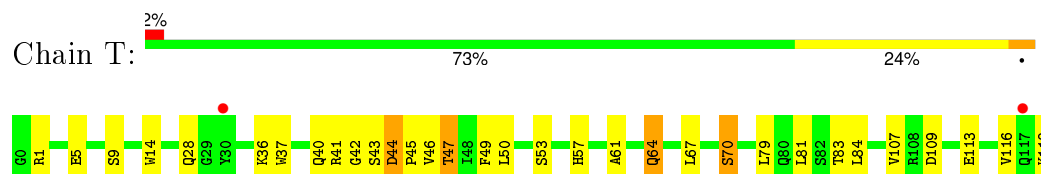SER ASN LEU D730 E731 D732 I733 I734 A735 E736 I739 R742 F745 W751 K757 E758 P759 P760 I771 F772 D775 S776 W780 L783 A784 V785 S786 M787 K790 K791 G792 I793 C794 V795 T802 D806 I809 L813 P814 Y815 S816 V817 V818 R819 N820 E821

Q822 V823 E824 V828 Q834 E837 L838 K839 V840 R841 V842 N847 F850 C851 S852 T855 Q861 P867 S871 L872 S873 V874 V877 I878 V879 P880 L881 K882 V890 V894 Y895 H896 H897 F898 I899 S900 D901 G902 L907 K908 V909 E912 GLY ILE ARG MET

ASN LYS THR VAL ALA VAL ARG THR LEU ASP PRO GLU ARG LEU GLY ARG

• Molecule 3: Complement C3 alpha chain

Chain C:

3%
56%　26%　14%

SER GLU GLU THR LYS GLU ASN GLU GLY PHE THR VAL THR ALA GLU GLY LYS GLY GLN GLY THR LEU SER VAL VAL THR MET TYR HIS ALA ALA LYS ALA LYS ASP GLN LEU T1335 C1336 N1337 K1338 F1339 D1340 L1341 K1342 V1343 T1344 P1347 A1348 P1349 GLU THR GLU LYS ARG PRO GLN ASP ALA K1359

N1360 T1361 M1362 I1363 L1364 R1369 Y1370 R1371 G1372 Q1374 D1375 A1376 T1377 M1378 L1381 T1393 N1401 G1402 V1403 D1404 I1407 L1412 D1413 K1414 R1419 I1424 Y1425 L1426 D1427 K1428 V1429 S1430 H1431 S1432 E1433 A1438 F1439 Y1444 F1445 I1450 Q1451 P1452 V1455 K1456 V1457 N1462

L1463 E1464 E1465 S1466 C1467 T1468 E1476 D1477 G1478 K1479 I1480 N1481 R1485 L1488 C1489 R1490 C1491 A1492 F1497 I1498 Q1499 K1500 SER ASP D1503 K1504 V1505 T1506 L1507 E1508 E1509 E1516 P1517 K1524 T1525 R1526 K1529 V1530 Q1531 L1532 S1533 N1534 M1541 E1544 S1551 Q1555 Q1558

S1564 P1565 I1566 K1567 K1573 E1576 H1579 Y1580 L1581 M1582 W1583 K1593 S1597 T1604 W1605 V1606 E1607 N1620 C1624 T1631 G1638 C1639 P1640 N1641

• Molecule 3: Complement C3 alpha chain

Chain F:

• Molecule 4: V-set and immunoglobulin domain-containing protein 4

Chain S:

• Molecule 4: V-set and immunoglobulin domain-containing protein 4

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	384.94Å 65.21Å 147.68Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.96 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-3.10) 95.3 (19.96-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.13 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.236 , 0.295 0.229 , 0.280	Depositor DCC
R_{free} test set	3112 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 62022 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19619	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, NAG

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	0.54	0/5108	0.67	0/6939
1	D	0.41	0/5004	0.59	0/6799
2	B	0.57	0/1512	0.66	0/2055
2	E	0.46	0/1512	0.59	0/2055
3	C	0.60	3/2453 (0.1%)	0.64	0/3305
3	F	0.38	0/2453	0.54	1/3305 (0.0%)
4	S	0.50	0/972	0.60	0/1323
4	T	0.41	0/972	0.64	1/1323 (0.1%)
All	All	0.49	3/19986 (0.0%)	0.62	2/27104 (0.0%)

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
1	A	0	3
1	D	0	3
2	B	0	1
3	C	0	1
4	S	0	1
4	T	0	2
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1607	GLU	CD-OE2	15.28	1.42	1.25
3	C	1607	GLU	CD-OE1	8.79	1.35	1.25
3	C	1620	ASN	CG-OD1	5.04	1.35	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	47	THR	N-CA-C	-9.05	86.56	111.00
3	F	1463	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ASP	Peptide
1	A	372	GLU	Peptide
1	A	40	PHE	Peptide
2	B	751	TRP	Peptide
3	C	1373	ASP	Peptide

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	5008	0	5071	116	0
1	D	4907	0	4971	97	0
2	B	1480	0	1502	32	0
2	E	1480	0	1502	38	0
3	C	2407	0	2321	66	0
3	F	2407	0	2321	42	0
4	S	950	0	935	20	0
4	T	950	0	935	12	0
5	A	28	0	25	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
All	All	19619	0	19583	384	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 10.

The worst 5 of 384 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:C:1370:TYR:O	3:C:1431:HIS:HB2	1.54	1.06
1:A:365:VAL:H	1:A:379:THR:HG22	1.22	1.02
1:D:365:VAL:H	1:D:379:THR:HG22	1.24	1.01
3:C:1516:GLU:HB3	3:C:1517:PRO:CD	1.98	0.93
4:S:44:ASP:HB2	4:S:45:PRO:HD3	1.51	0.91

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	640/642 (100%)	601 (94%)	23 (4%)	16 (2%)	7	32
1	D	624/642 (97%)	581 (93%)	27 (4%)	16 (3%)	7	32
2	B	181/206 (88%)	170 (94%)	9 (5%)	2 (1%)	17	55
2	E	181/206 (88%)	160 (88%)	20 (11%)	1 (1%)	30	68
3	C	290/343 (84%)	235 (81%)	42 (14%)	13 (4%)	3	17
3	F	290/343 (84%)	244 (84%)	35 (12%)	11 (4%)	4	22
4	S	117/119 (98%)	103 (88%)	13 (11%)	1 (1%)	21	61
4	T	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	7	32
All	All	2440/2620 (93%)	2194 (90%)	183 (8%)	63 (3%)	7	32

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	373	ASP
1	A	551	ARG
3	C	1373	ASP
3	C	1516	GLU

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	566/566 (100%)	499 (88%)	67 (12%)	6	25
1	D	555/566 (98%)	500 (90%)	55 (10%)	10	34
2	B	171/191 (90%)	157 (92%)	14 (8%)	14	47
2	E	171/191 (90%)	152 (89%)	19 (11%)	8	29
3	C	270/309 (87%)	234 (87%)	36 (13%)	5	20
3	F	270/309 (87%)	253 (94%)	17 (6%)	22	58
4	S	109/109 (100%)	100 (92%)	9 (8%)	14	46
4	T	109/109 (100%)	97 (89%)	12 (11%)	8	30
All	All	2221/2350 (94%)	1992 (90%)	229 (10%)	9	32

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1506	THR
1	D	26	ASP
3	F	1507	LEU
3	C	1564	SER
3	C	1631	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1462	ASN
4	S	28	GLN
4	T	59	GLN
3	C	1472	HIS
3	C	1558	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)

2 carbohydrates are 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	$\#|Z| > 2$
5	NAG	A	643	1,5	14,14,15	0.46	0	15,19,21	2.31	2 (13%)
5	NAG	A	644	5	14,14,15	0.51	0	15,19,21	0.81	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	NAG	A	643	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	644	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	643	NAG	C3-C4-C5	2.44	114.44	110.20
5	A	643	NAG	C1-O5-C5	8.11	122.54	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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	642/642 (100%)	-0.42	5 (0%)	87	75	17, 47, 84, 126	0
1	D	630/642 (98%)	0.24	36 (5%)	27	11	17, 50, 123, 142	0
2	B	183/206 (88%)	-0.59	1 (0%)	91	83	13, 37, 64, 82	0
2	E	183/206 (88%)	-0.28	3 (1%)	74	55	12, 49, 91, 95	0
3	C	296/343 (86%)	-0.14	9 (3%)	54	29	19, 60, 94, 116	0
3	F	296/343 (86%)	1.53	91 (30%)	1	0	42, 133, 199, 223	0
4	S	119/119 (100%)	-0.48	1 (0%)	87	75	22, 46, 68, 94	0
4	T	119/119 (100%)	-0.22	2 (1%)	73	52	22, 46, 68, 94	0
All	All	2468/2620 (94%)	0.02	148 (5%)	25	10	12, 51, 161, 223	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1610	PRO	12.8
3	F	1608	HIS	9.3
1	D	1	SER	7.2
3	F	1607	GLU	6.8
1	D	374	THR	6.8

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)

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(Å^2)	Q<0.9
5	NAG	A	643	14/15	0.95	0.16	-0.50	51,58,71,76	0
5	NAG	A	644	14/15	0.90	0.40	-	82,87,88,89	0

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(Å^2)	Q<0.9
6	CA	D	643	1/1	0.96	0.04	-2.26	64,64,64,64	0
6	CA	A	645	1/1	0.94	0.06	-2.62	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.