



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2A73
Title : Human Complement Component C3
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Deposited on : 2005-07-04
Resolution : 3.30 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

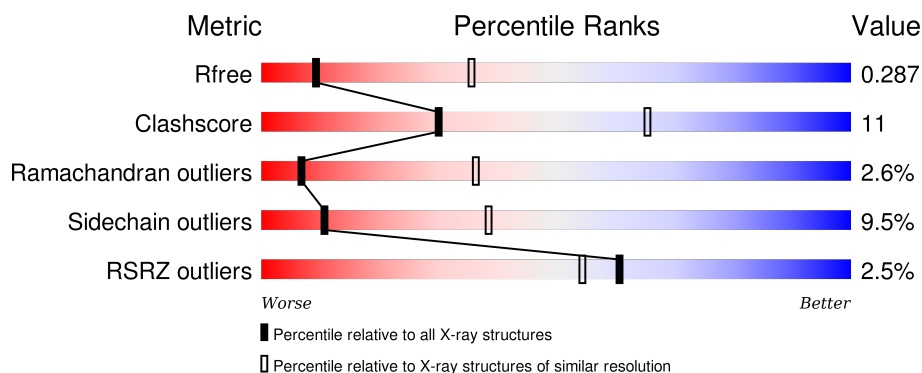
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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. 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	643	
2	B	991	

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
3	MAN	B	3	X	-	-	-
3	MAN	B	5	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12860 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	0	0
			4950	3153	837	945	15			

- Molecule 2 is a protein called Complement C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	976	Total	C	N	O	S	0	0	0
			7821	4943	1331	1501	46			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	5	Total	C	N	O	0	0
			61	34	2	25		

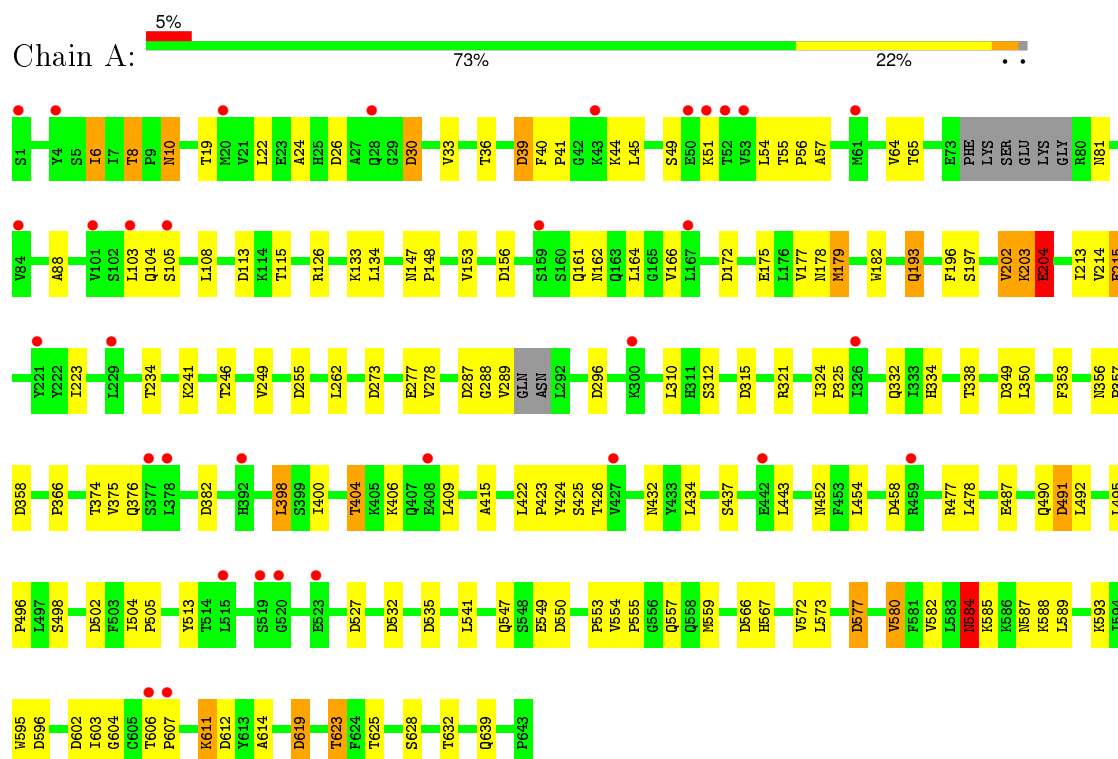
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

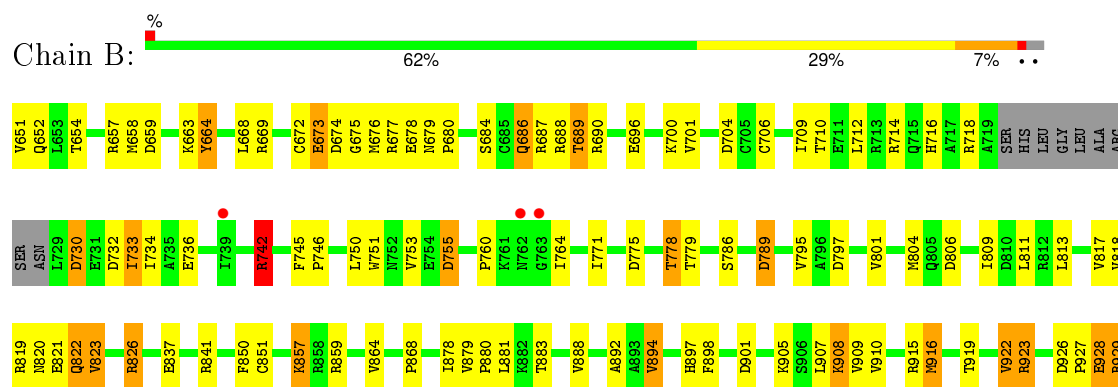
3 Residue-property plots

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



• Molecule 2: Complement C3



L930	D1007	A1120	Q1255	E1350	A1438	L1532
G931	E1008	L1121	A1256	T1351	F1439	E1544
R932	K1014	V1125	K1262	R1354	K1440	D1552
E933	L1126	L1126	D1263	P1355	Y1444	Q1555
G934	E1018	Q1130	D1266	Q1356	E1448	Q1558
K937	L1024	E1131	A1267	D1357	L1449	I1566
E938	K1029	A1132	Q1268	T1361	I1450	K1567
D939	K1033	K1133	E1269	Q1451	Q1451	C1568
I940	Q1033	D1134	L1270	R1371	V1457	K1577
D944	P1040	E1137	D1273	G1372	Y1460	W1583
D947	S1041	L1143	L1276	D1373	Y1460	D1588
Q948	S1042	P1144	Q1277	Q1374	Y1461	G1591
P950	A1043	I1147	L1278	D1375	M1462	E1592
D951	F1044	D1152	K1284	A1376	L1463	K1593
T952	P1052	D1157	I1285	T1377	E1464	P1594
E953	T1057	M1157	W1291	M1378	R1469	M1595
S954	S1065	I1169	E1292	S1379	P1473	L1596
E955	D1074	L1180	S1293	I1380	E1474	I1599
T956	Q1075	R1197	A1294	L1381	K1475	G1602
Q961	Q1076	D1200	S1295	D1382	K1476	D1603
G962	C1079	Q1204	L1302	M1385	D1477	T1604
T963	K1083	L1205	R1298	M1386	G1478	W1605
P964	K1091	Y1206	R1298	T1387	K1479	D1613
V965	P1092	V1208	T1302	P1390	L1480	D1617
A966	D1093	L1215	V1310	D1391	N1481	E1618
E970	G1094	Q1204	V1321	T1393	K1482	E1619
D971	V1095	L1205	V1322	D1394	L1483	D1626
D974	F1096	Y1207	T1324	D1395	C1484	E1632
H980	A1100	K1315	M1325	D1404	R1485	S1633
L981	D1099	V1208	Y1326	S1408	D1486	M1634
I982	I1103	L1215	H1327	K1409	C1489	N1641
V983	H1104	P1228	A1330	E1411	C1496	
P985	Q1105	P1229	D1332	L1412	F1497	
C988	E1106	Q1237	K1331	D1413	I1498	
G989	ILE	R1238	D1332	K1414	Q1499	
E990	GLY	Y1239	C1336	A1415	K1500	
Q991	GLY	Y1239	M1337	F1416	S1501	
I994	LEU	S1246	R1338	S1417	D1502	
G995	ARG	T1247	F1339	D1418	D1503	
T997	N1113	Q1248	L1341	R1419	E1509	
P998	M1114	A1249	I1423	M1420	D1512	
T999	M1115	T1250	I1424	I1423	E1516	
V1000	E1116	F1251	F1340	D1427	P1517	
I1001	K1117	M1252	D1340	K1428	G1518	
A1002	D1118	V1253	L1341	E1433	V1519	
Y1005	M1119	F1254	I1345	D1434	D1520	
L1006			P1347	D1435	K1524	
					L1527	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.98 Å 156.26 Å 271.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 39.12 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.30) 99.8 (39.12-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.32 Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.230 , 0.289 0.228 , 0.287	Depositor DCC
R_{free} test set	1882 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37699 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12860	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.21	0/5048	0.56	27/6859 (0.4%)
2	B	0.21	0/7973	0.59	54/10779 (0.5%)
All	All	0.21	0/13021	0.58	81/17638 (0.5%)

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	B	2	0

There are no bond length outliers.

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	602	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	674	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	730	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	1512	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	1413	ASP	CB-CG-OD2	5.49	123.25	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	3	MAN	C1
3	B	5	MAN	C1

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	4950	0	5012	83	0
2	B	7821	0	7743	211	0
3	B	61	0	52	4	0
4	A	28	0	25	0	0
All	All	12860	0	12832	286	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 11.

The worst 5 of 286 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:584:ASN:HB3	1:A:585:LYS:CA	1.85	1.07
1:A:584:ASN:CB	1:A:585:LYS:HA	1.84	1.06
2:B:908:LYS:HE3	2:B:1417:SER:HA	1.38	1.05
2:B:1484:CYS:HA	2:B:1489:CYS:HB2	1.37	1.04
1:A:584:ASN:HB3	1:A:585:LYS:HA	0.99	0.98

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	629/643 (98%)	564 (90%)	54 (9%)	11 (2%)	11	47
2	B	970/991 (98%)	853 (88%)	87 (9%)	30 (3%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1599/1634 (98%)	1417 (89%)	141 (9%)	41 (3%)	7	36

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	LYS
1	A	204	GLU
1	A	424	TYR
2	B	923	ARG
2	B	930	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	560/567 (99%)	525 (94%)	35 (6%)	22	60
2	B	867/878 (99%)	766 (88%)	101 (12%)	7	29
All	All	1427/1445 (99%)	1291 (90%)	136 (10%)	11	38

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	908	LYS
2	B	1024	LEU
2	B	1503	ASP
2	B	922	VAL
2	B	980	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	679	ASN
2	B	686	GLN
2	B	1472	HIS

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Mol	Chain	Res	Type
1	A	557	GLN
1	A	584	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

7 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	$\# Z > 2$
4	NAG	A	644	1,4	14,14,15	0.53	0	15,19,21	0.62	0
4	NAG	A	645	4	14,14,15	0.49	0	15,19,21	0.55	0
3	NAG	B	1	3,2	14,14,15	0.60	0	15,19,21	1.17	2 (13%)
3	NAG	B	2	3	14,14,15	0.65	0	15,19,21	1.17	1 (6%)
3	MAN	B	3	3	11,11,12	0.81	0	14,15,17	0.71	0
3	BMA	B	4	3	11,11,12	0.62	0	14,15,17	0.76	1 (7%)
3	MAN	B	5	3	11,11,12	0.61	0	14,15,17	0.66	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
4	NAG	A	644	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	645	4	-	2/6/23/26	0/1/1/1
3	NAG	B	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	MAN	B	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	BMA	B	4	3	-	0/2/19/22	0/1/1/1
3	MAN	B	5	3	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4	BMA	C1-C2-C3	2.06	111.97	109.54
3	B	1	NAG	C3-C4-C5	2.45	114.47	110.20
3	B	1	NAG	C4-C3-C2	2.66	115.36	111.23
3	B	2	NAG	C4-C3-C2	3.67	116.94	111.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	3	MAN	C1
3	B	5	MAN	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	645	NAG	C8-C7-N2-C2
4	A	645	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	NAG	3	0
3	B	3	MAN	1	0
3	B	5	MAN	1	0

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	635/643 (98%)	0.36	33 (5%) 31 25	79, 97, 116, 123	0
2	B	976/991 (98%)	0.08	8 (0%) 87 84	71, 91, 108, 129	0
All	All	1611/1634 (98%)	0.19	41 (2%) 61 54	71, 93, 113, 129	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	MET	3.8
1	A	101	VAL	3.8
2	B	739	ILE	3.8
1	A	427	VAL	3.5
1	A	61	MET	3.3

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
4	NAG	A	645	14/15	0.62	0.32	-	106,106,106,107	0
3	NAG	B	2	14/15	0.89	0.19	-	126,129,132,138	0
3	BMA	B	4	11/12	0.60	0.31	-	150,151,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MAN	B	3	11/12	0.84	0.19	-	141,144,147,149	0
3	NAG	B	1	14/15	0.90	0.22	-	109,113,116,121	0
4	NAG	A	644	14/15	0.71	0.30	-	107,108,108,109	0
3	MAN	B	5	11/12	0.68	0.33	-	147,148,148,149	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.