



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID : 2B39
Title : Structure of mammalian C3 with an intact thioester at 3Å resolution
Authors : Fredslund, F.; Jenner, L.; Husted, L.B.; Nyborg, J.; Andersen, G.R.; Sottrup-Jensen, L.
Deposited on : 2005-09-20
Resolution : 3.00 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

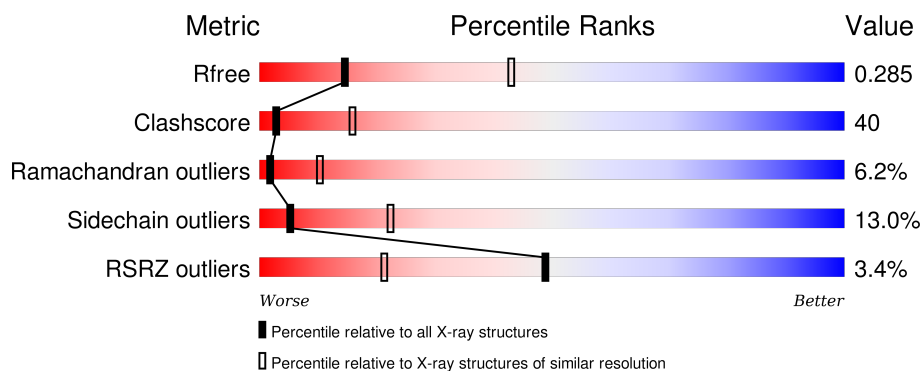
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	1661	<div> <div>4%</div> <div>39%</div> <div>46%</div> <div>11%</div> <div>..</div> </div>
1	B	1661	<div> <div>3%</div> <div>38%</div> <div>48%</div> <div>10%</div> <div>..</div> </div>

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
2	NAG	A	2001	X	-	-	-
2	NAG	B	2001	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25624 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 C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1610	Total	C	N	O	S	0	0	0
			12773	8093	2187	2439	54			
1	B	1610	Total	C	N	O	S	0	0	0
			12773	8093	2187	2439	54			

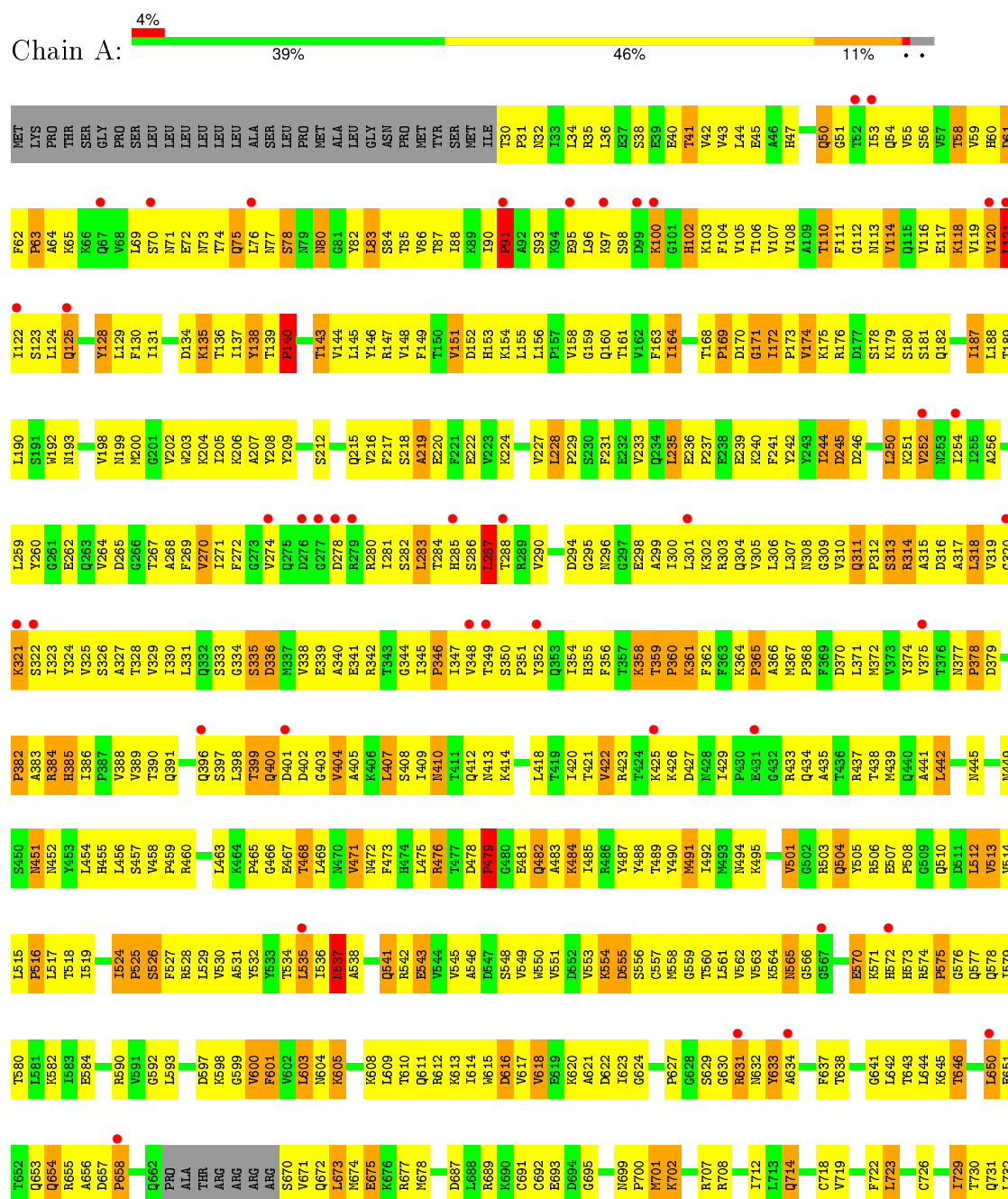
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

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 ($\text{RSRZ} > 2$). 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: C3





R1133	D1028	T927	R360	L794	C725	Q659	R598	R528	P459	Q396	G334	A268	T189	S126
D1134	W1033	L928	V861	K795	C726	C660	G599	L529	R460	S397	G334	F269	T189	G127
T1135	W1033	R929	R862	D796		P661	V600	V530	V461	L398	S335	V270	L190	Y128
R1136	E1034	V930	V863	S797		Q662		A531	E462	T399	D336	I271	W192	L129
E1137	K1035	V931	E864	S798	I729	P80	L603	Y532	K463	Q400	R337	G272		F130
R1242	E1039	P932	L665	T799	Q731	ALA	R604	Y533	K464	D401		G273	L197	I131
K1243	E1040	E933	L666	T800	Q732	THR	K605	T534	P465	D402		V274	V198	Q132
D1244	R1041		V867	W801	R733	ARG	R607	L535	G466	G403		D275	M199	T133
	S1141	T940		E802	Q734	ARG		L536	V404	V403		D276	M200	D134
T1247	Q1042	T945	A870	L804	H735	ARG		N537	E467			G277		T135
P1249	S1044	L946	F871	A805	H736	ARG		A538	T343	K405		D278	W203	K135
P1250	L1045		C572	R806		ARG		A539	L469	K406		R279	K204	T136
	E1046	R958	T876	S807	L742	S870	T610	K539	N470	L407		R280	K204	I137
L1255	L1047		A877	L808	L743	V871	R611	K540	V471	S408		R281	I205	Y138
E1257	L1048	V961	A878		L744	Q872	R612	G540	N472	I409		I281		T139
Q1258	R1049	P962	K811	L808	GLU	L673	R613	R542	N410			S282	Y208	P140
R1259	R1049		R812		ALA	M674	T614	V545	L475	N413		L283		T143
Y1260	R880		G813		ARG	E875	W615		R476	K414		T284	Q213	V144
	R881		I814		ARG	K676	D616		D478	P351		R285	Q214	T145
Y1261		D872			ASP	R677	V617		P479	R415		S286	Q215	L146
			T885		LEU		W618		G480	D416		L287	V216	Y146
Y1265	E976	E976	T886			K680	W550		E481			T288	F217	R147
G1266	T977	T977	I887	A817	D751	Q683	W551		Q482			R289	A219	F148
S1267	K1061	Q982	P888	D818	D752	D622	A621		A483	V422		V290		
T1268	A1064			P819	I753	I623	K634		R423	K357			K224	T150
Q1269		P985	S891	R820	I754	G624	L485		T424	K358		G295	E225	V151
A1270	P1073	Y986	S892	E821	P755	C625	L486		K425	T359		I296	E225	D152
T1271	A894	A987	V893	R822	E756	T626	Y487		K426			G297	Y226	H153
F1272	L1077	Q988	T823	T823	E757	P637	Y488		R426			E298	V227	K154
M1273	T1078	N989	W825	M825		G628	T489		N428	F362		L228	P229	L155
V1274		T990	Q826		S761	S629	L561		I429	F363		A299		L156
F1275	V1081	E991	V898		S762	G630	M491		P430	K364		I300		P157
A1191	V1082	D992	R899	F829	S763	R631	M492		E431	P365		I301	Q234	V158
Y1193	A1086	A993	V900	L834	Q764	N632	L492		G432			R302	L235	G159
A1194		D995	P901	D831	P765	K564	M493		R433			R303	E236	T160
L1201	L1091	G996	T904	L832	E767	A634			Q434			Q304	P237	T161
E1202	I1092	E997	G905	R833	S768	G635			L498			V305	E238	V162
Q1282	A1093	R998	L906	L834	W769				L499			L306	E239	F163
K1283	I1094	L999	H907	P835	W771				A435			L307	K240	T164
D1284	D1095		E908	V838	T772	Q706			A435			L308	F241	T165
V1285	D1098		V909	R839	T773	R707	G641		R506			G309	Y242	T166
P1286	I1003		E910	R840	T774	R708	L642		A441			Q311	I244	T168
D1287	Q1004		V911	R841		A709	T643		E507			P312	D245	P169
H1288	I1107		K912	E842		A709	T643		P508			D316	D246	D170
K1289	L1108		A913	R843	L777	F703	Q578		Y444			A317	P247	G171
E1290	L1109		G914	Q843	K778	F704	Q578		G509			A317	D248	I172
K1291	G1010		R844	P844	Q779	T711	L579		N445			L318	G249	P173
L1296	E1011		V915	E845	A780	I712	T580		T446			V319	L250	V174
P1297	Q1012		Y916	I846	D781	L713	L581		Q447			G320	K251	K175
			R917	R847	T782	Q714	Q648		G448			K321		R176
			H918	A848	K782	G715	G649		N449			S322	A256	
			P919	R849	Q784	Q710	L650		S460			I323	R257	S180
			I920	L850	I785	F717	B651		I519			Y324	F258	S181
	P1019		S921	Y851	S786	Q718	T520		N451			V325	F259	Q182
			D822	N852	T787	V719	Q653		N452			L259	Y260	L183
			G923	R853		Q654	R590		Y453			S326		Q184
			R854	R854			G592		L454			A327		T185
							L593		L456			V329		G186
							D597		S457			I330		I187
									V458			L331		L188



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	254.25Å 246.86Å 113.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 37.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 97.2 (37.85-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.278 , 0.286 0.273 , 0.285	Depositor DCC
R_{free} test set	1392 reflections (1.00%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.6	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 138964 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25624	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.58	1/13020 (0.0%)	0.82	15/17632 (0.1%)
1	B	0.57	0/13020	0.81	11/17632 (0.1%)
All	All	0.57	1/26040 (0.0%)	0.82	26/35264 (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
1	A	0	1
1	B	0	1
2	A	1	0
2	B	1	0
All	All	2	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	HIS	CB-CG	6.64	1.61	1.50

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	LEU	CA-CB-CG	-9.75	92.87	115.30
1	A	91	PRO	N-CA-C	7.91	132.66	112.10
1	B	1362	LEU	CA-CB-CG	6.57	130.40	115.30
1	A	1362	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	1130	GLY	N-CA-C	-6.49	96.87	113.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	NAG	C1
2	B	2001	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
1	B	820	TYR	Sidechain

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	12773	0	12782	1027	0
1	B	12773	0	12782	1002	0
2	A	39	0	34	3	0
2	B	39	0	34	3	0
All	All	25624	0	25632	2029	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 40.

The worst 5 of 2029 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:117:GLU:O	1:B:118:LYS:HG2	1.47	1.14
1:B:369:PHE:HB3	1:B:409:ILE:HD12	1.32	1.10
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.34	1.09
1:B:244:ILE:HD11	1:B:319:VAL:CG2	1.84	1.08
1:B:116:VAL:HG13	1:B:645:LYS:HG2	1.28	1.06

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	1602/1661 (96%)	1285 (80%)	213 (13%)	104 (6%)	1	8
1	B	1602/1661 (96%)	1268 (79%)	239 (15%)	95 (6%)	2	11
All	All	3204/3322 (96%)	2553 (80%)	452 (14%)	199 (6%)	2	10

5 of 199 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	91	PRO
1	A	187	ILE
1	A	212	SER
1	A	244	ILE

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	1420/1465 (97%)	1238 (87%)	182 (13%)	5	23
1	B	1420/1465 (97%)	1234 (87%)	186 (13%)	5	22
All	All	2840/2930 (97%)	2472 (87%)	368 (13%)	5	22

5 of 368 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1447	ASP

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Mol	Chain	Res	Type
1	B	151	VAL
1	B	1351	LEU
1	A	1492	HIS
1	B	54	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	71	ASN
1	B	296	ASN
1	B	1298	GLN
1	B	79	ASN
1	B	184	GLN

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 ⓘ

6 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	$\# Z > 2$
2	NAG	A	2001	1,2	14,14,15	0.56	0	15,19,21	0.78	0
2	NAG	A	2002	2	14,14,15	0.61	0	15,19,21	1.01	1 (6%)
2	BMA	A	2003	2	11,11,12	0.46	0	14,15,17	0.49	0
2	NAG	B	2001	1,2	14,14,15	0.57	0	15,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	2002	2	14,14,15	0.60	0	15,19,21	0.89	0
2	BMA	B	2003	2	11,11,12	0.47	0	14,15,17	0.67	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
2	NAG	A	2001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	2003	2	-	0/2/19/22	0/1/1/1
2	NAG	B	2001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
2	BMA	B	2003	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	NAG	C3-C4-C5	-2.37	106.06	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	NAG	C1
2	B	2001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	NAG	3	0
2	A	2002	NAG	2	0
2	B	2001	NAG	1	0
2	B	2002	NAG	2	0
2	B	2003	BMA	1	0

5.6 Ligand geometry [i](#)

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	1610/1661 (96%)	-0.04	59 (3%)	45	19	15, 101, 169, 200	0
1	B	1610/1661 (96%)	-0.10	51 (3%)	51	23	17, 96, 169, 200	0
All	All	3220/3322 (96%)	-0.07	110 (3%)	49	21	15, 99, 169, 200	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	671	VAL	6.0
1	A	742	LEU	5.9
1	A	741	ALA	5.2
1	A	276	ASP	5.0
1	A	348	VAL	5.0

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
2	NAG	A	2001	14/15	0.83	0.24	1.06	74,80,81,82	0
2	NAG	B	2002	14/15	0.88	0.26	0.81	80,80,81,82	0
2	BMA	A	2003	11/12	0.72	0.40	-	81,81,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	2002	14/15	0.80	0.32	-	80,81,82,82	0
2	NAG	B	2001	14/15	0.93	0.15	-	73,80,81,82	0
2	BMA	B	2003	11/12	0.79	0.23	-	80,81,81,82	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.